HIGH-END COMPUTING CAPABILITY PORTFOLIO

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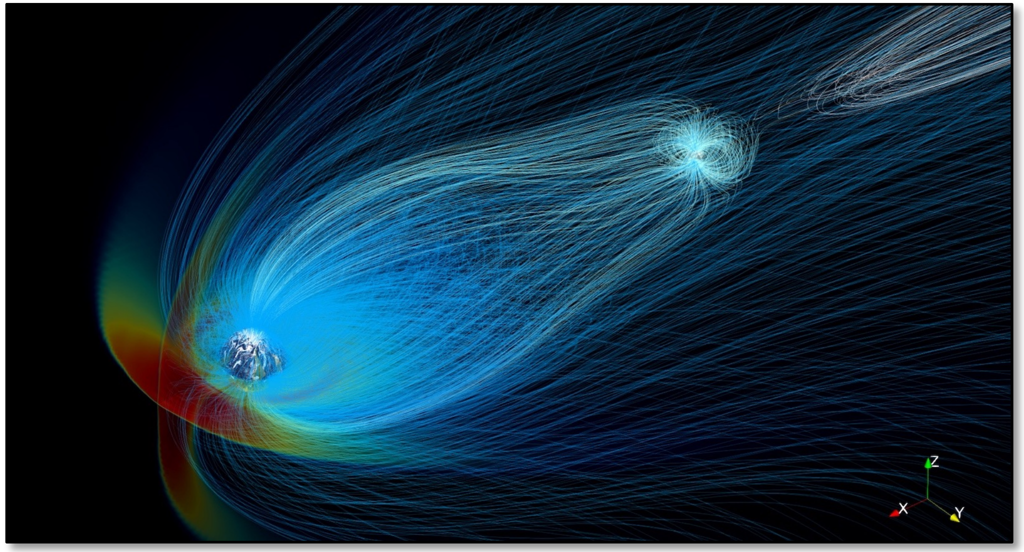
National Aeronautics and Space Administration

HECC Supercomputer Usage Sets New Record

- In January 2022, the combined usage of HECC supercomputers set a new record of 12,516,376 Standard Billing Units (SBUs).*
- The usage by 394 of NASA's science and engineering groups exceeded the previous record of 12,338,448 SBUs set in July 2021 by 177,928 SBUs.
- The record was achieved in great part by two projects from the Science Mission Directorate's Earth Science Division:
  - Coupled Goddard Earth Observing System (GEOS)/Estimating the Circulation and Climate of the Ocean (ECCO)
  - Astrophysics Roles of Stellar Flares and Storms in Exoplanetary Atmospheric Losses and Evolution
- Usage of Pleiades, Aitken, Electra, Merope, and Endeavour contributed to this record. The new record was enabled by the Aitken Rome nodes, with 128 cores per node.
- The top 10 projects' usage ranged between 215,245 and 1,159,239 SBUs and together accounted for over 36% of the total usage.
- The HECC Project continues to evaluate and plan resources to address the future requirements of NASA's users.

** 1 SBU represents the work that can be done in 1 hour on a Pleiades Broadwell 28-core node.*

IMPACT: The increased capacity of HECC systems and working with users to optimize their run capacities provides mission directorates with more resources to accomplish their goals and objectives.



3D representation of the entire magnetized Earth-Moon system during an extreme "Carrington-type" space weather event, where the moon is in the wake of the Earth. Color contours depict the total fluid pressure in nanoscale, while the cyan lines represent magnetic fields through which oxygen ions can be transported from Earth to the lunar poles. *Chuanfei Dong, Liang Wang, Princeton University*

TOSS Replaces SuSE on Compute Nodes

- HECC teams completed the transition of the default operating system for most systems from the SuSE Linux Enterprise Server (SLES) to the Linux-based Tri-Lab Operating System Stack (TOSS) developed and maintained by Department of Energy (DOE) Labs. TOSS is designed for efficiently running large-scale HPC workloads.
- TOSS 3 is a Red Hat Enterprise Linux (RHEL)-based operating system optimized for HPC clusters. The biggest challenge of the migration from SLES12 to TOSS3 was validating the new software environment that HECC users rely on.
- Extensive TOSS testing was conducted to identify and remediate software compatibility and workflow issues to ensure a minimal impact on the user community from the migration.
- HECC is leveraging past and future DOE HPC work in operating systems and application scaling. HECC will join with the existing organizations utilizing TOSS to contribute improvements to the TOSS kernel.
- With access to TOSS kernel build environment, HECC can incorporate our local modules into the build environment, and our software build process will improve and become more efficient.

IMPACT: Migrating to TOSS 3, which is optimized for high-performance computing clusters, can reduce the total cost of ownership, enable application portability, and ensure timely access to security patches for HECC systems.

Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

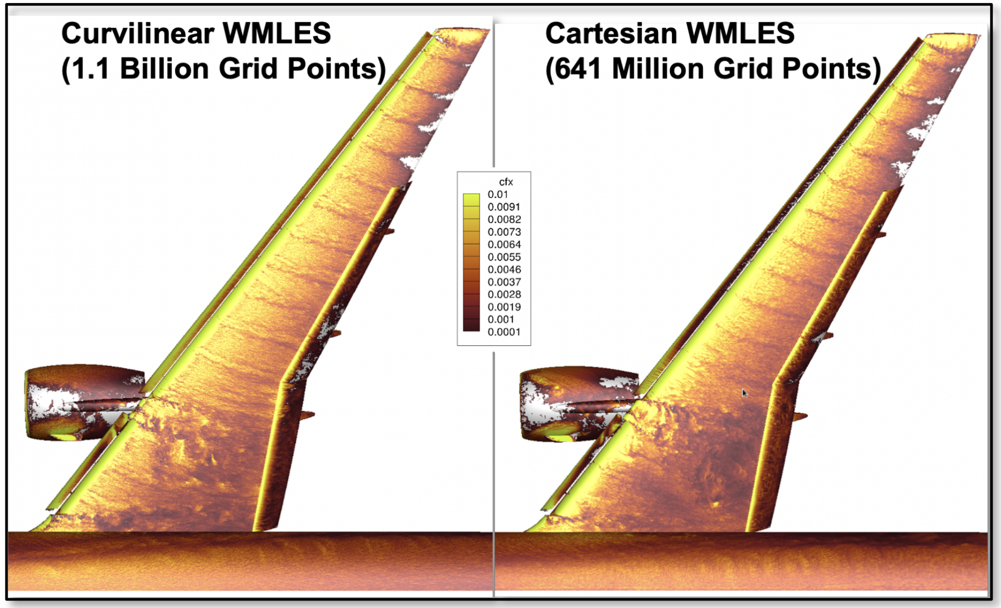
Sandia National Laboratories

The original TOSS environment effort was led by Lawrence Livermore National Laboratory (LLNL) and was built as a common capacity hardware environment, called the Tri-Lab Linux Capacity Clusters (TLCC1), at the three National Nuclear Security Administration laboratories: LLNL, Los Alamos, and Sandia.

LAVA WMLES Studies of the High-Lift CRM on HECC Cloud

- Utilizing the HECC Cloud to access Amazon Web Services (AWS) resources, in addition to in-house HECC resources, the LAVA team carried out Wall-Modeled Large Eddy Simulation (WMLES) studies of the High-Lift Common Research Model (HL-CRM) and met important deadlines for the AIAA Scitech CFD 2030 special session and the High-Lift Prediction Workshop data submission.
- The team found that per-node performance and interconnect of AWS resources are comparable to or even better than HECC systems. In addition:
  - Up to 160 c5n-type AWS nodes were utilized, with the queue wait time never exceeding five minutes.
  - Visualization and post-processing can both be completed in the cloud, eliminating the need for large data transfers and dedicated post-processing workstations.
  - On-demand cloud resources are approximately 5-8 times more expensive than in-house HECC resources.
- Evaluation of other node types, such as p4d (with 8xA100 GPUs) is planned for 2022 to facilitate rapid development and debugging of LAVA GPU capabilities, perform scaling studies, and provide feedback to HECC management.

IMPACT: Availability of on-demand HECC Cloud resources enables important NASA applications to be performed in a timely matter in order to meet critical milestones.

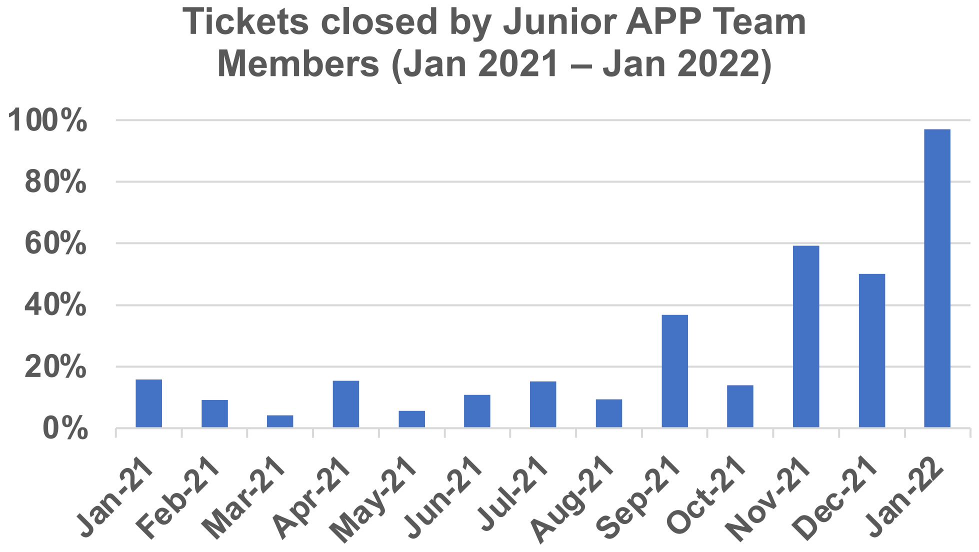


Instantaneous surface skin friction (c_{fx}) at (CL_{max}) predicted from LAVA for two WMLES cases utilizing AWS resources and in-house HECC resources. *Gaetan Kenway, Aditya Ghate, NASA/Ames*

APP Team Implements Three-Tier Support Structure

- Starting in late November, HECC's Application Performance and Productivity (APP) team moved from a two-tier support structure to three tiers. The new structure includes the Control Room (Tier I), junior APP team members (Tier II), and senior APP team members (Tier III). The change has the following goals:
  - Expose Tier II to end-user issues and solutions daily to accelerate their training.
  - Allow Tier III to focus on longer term projects and more complicated end-user issues.
- After two months the transition is going smoothly.
  - Members of Tier II reported an improved understanding of common end user issues and their corresponding solutions.
  - There were 136 tickets closed from Nov. 2020-Jan. 2021 (~16% closed by junior staff) and 276 tickets closed from Nov. 2021-Jan. 2022 (~65% closed by junior staff). This is above average for APP (normally ~75 tickets per month), but the team is handling the higher load well.
  - There are currently fewer than 50 open tickets.
- It is expected that the cumulative exposure of Tier II to end-user issues in the coming months will result in increased Tier II autonomy, more Tier III availability for complex and long-term projects, and improved efficiency beyond what was seen previously under the two-tier support structure.

IMPACT: Implementing a three-tier support structure can improve efficiency by allowing senior team members to focus on longer term research projects.

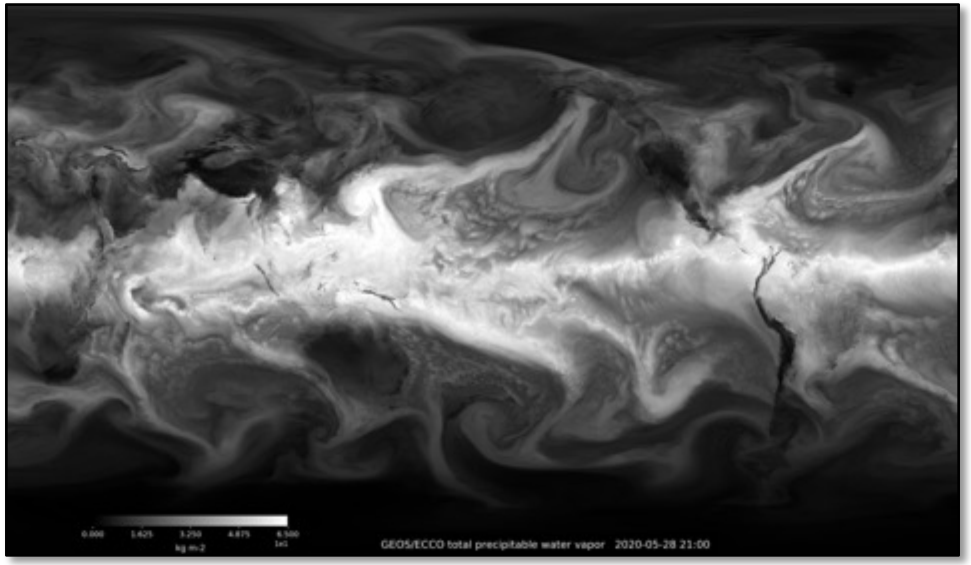


Since starting APP's three-tier support model in November, junior staff ticket closures have increased significantly. *Evan Dodge, ASRC Federal.*

High-Resolution Global Coupled GEOS-ECCO Simulation*

- Earth scientists at NASA JPL, NASA Ames, and MIT are using HECC supercomputers to advance NASA's oceanic and atmospheric estimation and prediction capability by combining the agency's flagship modeling and data assimilation efforts: the Goddard Earth Observing System (GEOS) and the Estimating the Circulation and Climate of the Ocean (ECCO) models.
  - The team's high-resolution, global coupled model provides a much more realistic description of air-sea interactions and oceanic and atmospheric planetary boundary layers than previously available in the separate models.
  - The coupled model helps researchers understand how ocean eddies—a major pathway for transferring heat from the ocean to the atmosphere—affect both air and sea circulation.
  - One analysis revealed three-to-six-day oscillations of sea surface temperatures and surface wind anomalies, a phenomenon appearing in observational records and reanalyses but previously unseen in ocean-only simulations.
- Insights gained from this work will help explain how these complex processes work together and will improve understanding of Earth's climate and weather, and how both are changing.

IMPACT: These large, complex global climate simulations improve our understanding of air-sea interactions and the effects of global changes; and support the development and utilization of existing and future NASA earth observing satellite missions.



Video showing total precipitable water, revealed by a coupled ocean-atmosphere simulation with kilometer-scale resolution. Low- (black) to high- (white) column water vapor content is shown, with spatial variability on many scales, from small cloud clusters to large-scale atmospheric rivers. *Nina McCurdy, David Ellsworth, NASA/Ames*

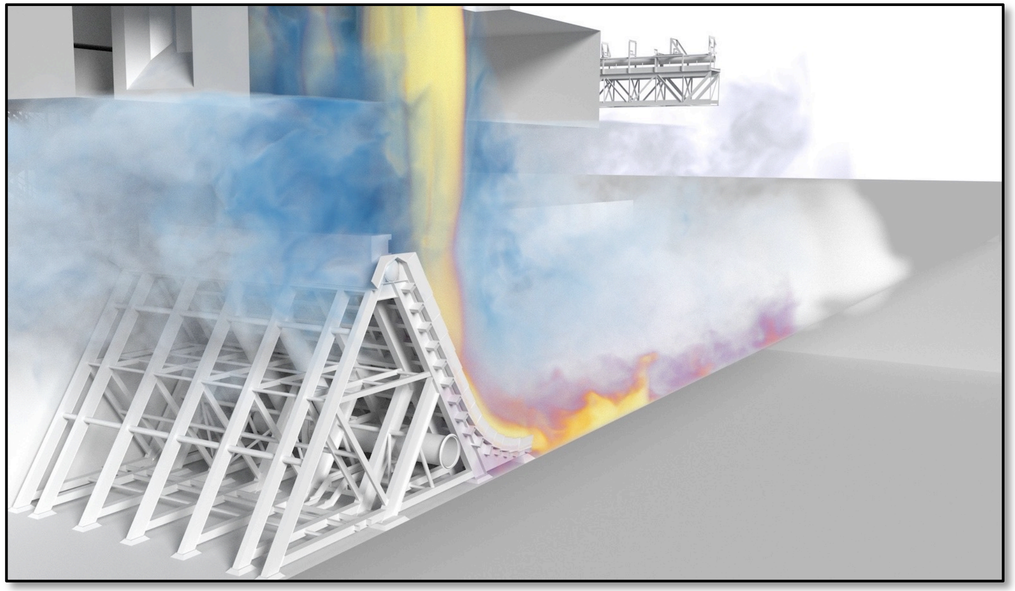
** HECC provided supercomputing resources and services in support of this work.*

Simulating the Launch Environment at NASA KSC*

- To support upcoming NASA Artemis missions from Kennedy Space Center's (KSC) Launch Complex 39B, the Launch Ascent and Vehicle Aerodynamics (LAVA) team in the NASA Advanced Supercomputing Division developed a new computational fluid dynamics (CFD) approach to accurately simulate the launch environment, including the water-based sound suppression system.
- Starting in 2020, KSC Exploration Ground Systems supported the utilization of LAVA's multiphase flow simulation capabilities to study the extreme conditions computationally, including modeling the Scale Model Acoustic Test (SMAT), a 5% scale test meant to represent the Space Launch System and Mobile Launcher. LAVA simulations of the SMAT were compared to pressure signals across various locations in the test environment and showed excellent agreement.
- Additionally, the team is using LAVA to provide ignition overpressure protection estimates for Launch Complex 39B and generating more accurate predictions by refining the model to include the sound suppression system's water effects.
- Each simulation required 400–500 million grid cells and ran several weeks on 8,000 cores of the Electra supercomputer's Skylake or Aitken's Cascade Lake processors. Nearly 400 terabytes of data were generated for each run.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: The multiphase results and new computational capabilities from this work will give the agency a better understanding of the extreme conditions of the launch environment, helping to reduce risk and increase safety.



This video depicts the Space Launch System's geometry and a volume rendering of mass fractions for liquid water (blue), water vapor (white), and vehicle exhaust (purple low, yellow high). The water system and liquid engines are started and allowed to reach a quasi-steady state before the solid motor engines are started. *Scott Neuhoff, Timothy Sandstrom (NASA/Ames)*

Papers

- "**Do We Need to Consider Electron Kinetic Effects to Properly Model a Planetary Magnetosphere: The Case of Mercury**," G. Lapenta, et al., arXiv:2201.01653 [astro-ph.EP], January 5, 2022. *
  https://arxiv.org/abs/2201.01653
- "**Magnetic Fields in the Formation of the First Stars.—II Results**," A. Stacy, et al., arXiv:2201.02225 [astro-ph.CO], January 6, 2022. *
  https://arxiv.org/abs/2201.02225
- "**Stochastic Low-Frequency Variability in the Three-Dimensional Radiation Hydrodynamical Models of Massive Star Envelopes**," W. Schultz, et al., The Astrophysical Journal Letters, vol. 924, no. 1, January 6, 2022. *
  https://iopscience.iop.org/article/10.3847/2041-8213/ac441f/meta
- "**Evolution of High-Frequency Instabilities in the Presence of Azimuthally Compact Crossflow Vortex Pattern over a Yawned Cone**," M. Choudhari, et al., Theoretical and Computational Fluid Dynamics (Springer), January 6, 2022. *
  https://link.springer.com/article/10.1007/s00162-021-00594-8
- "**Impacts of Lower Thermospheric Atomic Oxygen and Dynamics on the Thermospheric Semiannual Oscillation using GITM and WACCM-X**," G. Malhotra, et al., Journal of Space Physics, published online January 6, 2022. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2021JA029320
- "**TOI-2257 b: A Highly Eccentric Long-Period Sub-Neptune Transiting a Nearby M-Dwarf**," N. Schanche, et al., Astronomy & Astrophysics, vol. 657, January 7, 2022. *
  https://www.aanda.org/articles/aa/full_html/2022/01/aa42280-21/aa42280-21.html

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Papers (cont.)

- “**Laboratory Simulation of Solar Wind Interaction with Lunar Magnetic Anomalies**,” L. H. Yeo, et al., Journal of Geophysical Research: Space Physics, vol. 127, issue 1, January 10, 2022. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021JA029821
- “**TESS Giants Transiting Giants. I.: A Noninflated Hot Jupiter Orbiting a Massive Subgiant**,” N. Saunders, et al., The Astronomical Journal, vol. 163, no. 2, January 10, 2022. *
https://iopscience.iop.org/article/10.3847/1538-3881/ac38a1/meta
- “**TESS Giants Transiting Giants. II.: The Hottest Jupiters Orbiting Evolved Stars**,” S. Grunblatt, et al., arXiv:2201.04140 [astro-ph.EP], January 11, 2022. *
https://arxiv.org/abs/2201.04140
- “**Simultaneous High Dynamic Range Algorithm, Testing, and Instrument Simulation**,” J. Mason, et al., The Astronomical Journal, vol. 924, no. 2, January 12, 2022. *
https://iopscience.iop.org/article/10.3847/1538-4357/ac33a1/meta
- “**Black Hole – Galaxy Scaling Relations in FIRE: The Importance of Black Hole Location and Mergers**,” O. Çatmabacak, et al., Monthly Notices of the Astronomical Society, published online January 12, 2022. *
https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/stac040/6505143
- “**A Pair of Sub-Neptunes Transiting the Bright K-Dwarf TOI-1064 Characterized with *CHEOPS***,” T. Willson, et al., Monthly Notices of the Royal Astronomical Society, published online January 13, 2022. *
https://academic.oup.com/mnras/advance-article/doi/10.1093/mnras/stab3799/6506474?login=true

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Papers (cont.)

- “**Data-Driven Expectations for Electromagnetic Counterpart Searches Based on LIGO/Virgo Public Alerts**,” P. Petrov, The Astrophysical Journal, vol. 924, no. 2, January 12, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ac366d
- “**The TESS-Keck Survey. VIII. Confirmation of a Transiting Giant Planet on an Eccentric 261 Day Orbit with the Automated Planet Finder Telescope**,” P. Dalba, et al., The Astronomical Journal, vol. 163, no. 2, published January 13, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-3881/ac415b/meta
- “**An Exomoon Survey of 70 Cool Giants Exoplanets and the New Candidate Kepler-1708b-I**,” D. Kipping, et al., Nature Astronomy, published online January 13, 2022. *
  https://www.nature.com/articles/s41550-021-01539-1
- “**Satellite Observation of Stratospheric Intrusions and Ozone Transport using CrIS on SNPP**,” X. Xiong, et al., Atmospheric Environment, published online January 15, 2022. *
  https://www.sciencedirect.com/science/article/pii/S1352231022000218
- “**The Solar Wind with Hydrogen Ion Exchange and Large-scale Dynamics (SHIELD) Code: A Self-Consistent Kinetic-Magnetohydrodynamic Model of the Outer Heliosphere**,” A. Michael, et al., The Astrophysical Journal, vol. 924, no. 2, January 17, 2022. *
  https://iopscience.iop.org/article/10.3847/1538-4357/ac35eb/meta

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Papers (cont.)

- “**Influence of Nonseasonal River Discharge on Sea Surface Salinity and Height**,” H. Chandanpurkar, et al., Journal of Advances in Modeling Earth Systems, vol. 14, issue 2, January 18, 2022. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021MS002715
- “**Updraft Dynamics and Microphysics: On the Added Value of the Cumulus Thermal Reference Frame in Simulations of Aerosol-Deep Convection Interactions**,” D. Hernandez-Deckers, et al., Atmospheric Chemistry and Physics, vol. 22, issue 2, January 19, 2022. *
https://acp.copernicus.org/articles/22/711/2022/
- “**Investigating the Architecture and Internal Structure of the TOI-561 System Planets with CHEOPS, HARPS-N and TESS**,” G. Lacedelli, et al., arXiv:2201.07727 [astro-ph.EP], January 19, 2022. *
https://arxiv.org/abs/2201.07727
- “**An Extended and Fragmented Alfvén Zone in the Young Solar Wind**,” R. Chhiber, et al., arXiv:2201.08422 [astro-hSR], January 20, 2022. *
https://arxiv.org/abs/2201.08422
- “**TESS Revisits WASP-12: Updated Orbital Decay Rate and Constraints on Atmospheric Variability**,” I. Wong, et al., arXiv:2201.08370 [astro-ph.EP], January 20, 2022. *
https://arxiv.org/abs/2201.08370

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Papers (cont.)

- "**Structure of the Thermal Boundary Layer in Turbulent Channel Flows at Transcritical Conditions**," J. Guo, et al., Journal of Fluid Mechanics, vol. 934, January 21, 2022. *
  https://www.cambridge.org/core/journals/journal-of-fluid-mechanics/article/abs/structure-of-the-thermal-boundary-layer-in-turbulent-channel-flows-at-transcritical-conditions/CFC64179110D2AE4D25088925FCBD5E2
- "**Probing Multiphase Gas in Local Massive Elliptical Galaxies via Mulltiwavelength Observations**," P. Temi, et al., arXiv:2201.09330 [astro-ph.GA], January 23, 2022. *
  https://arxiv.org/abs/2201.09330

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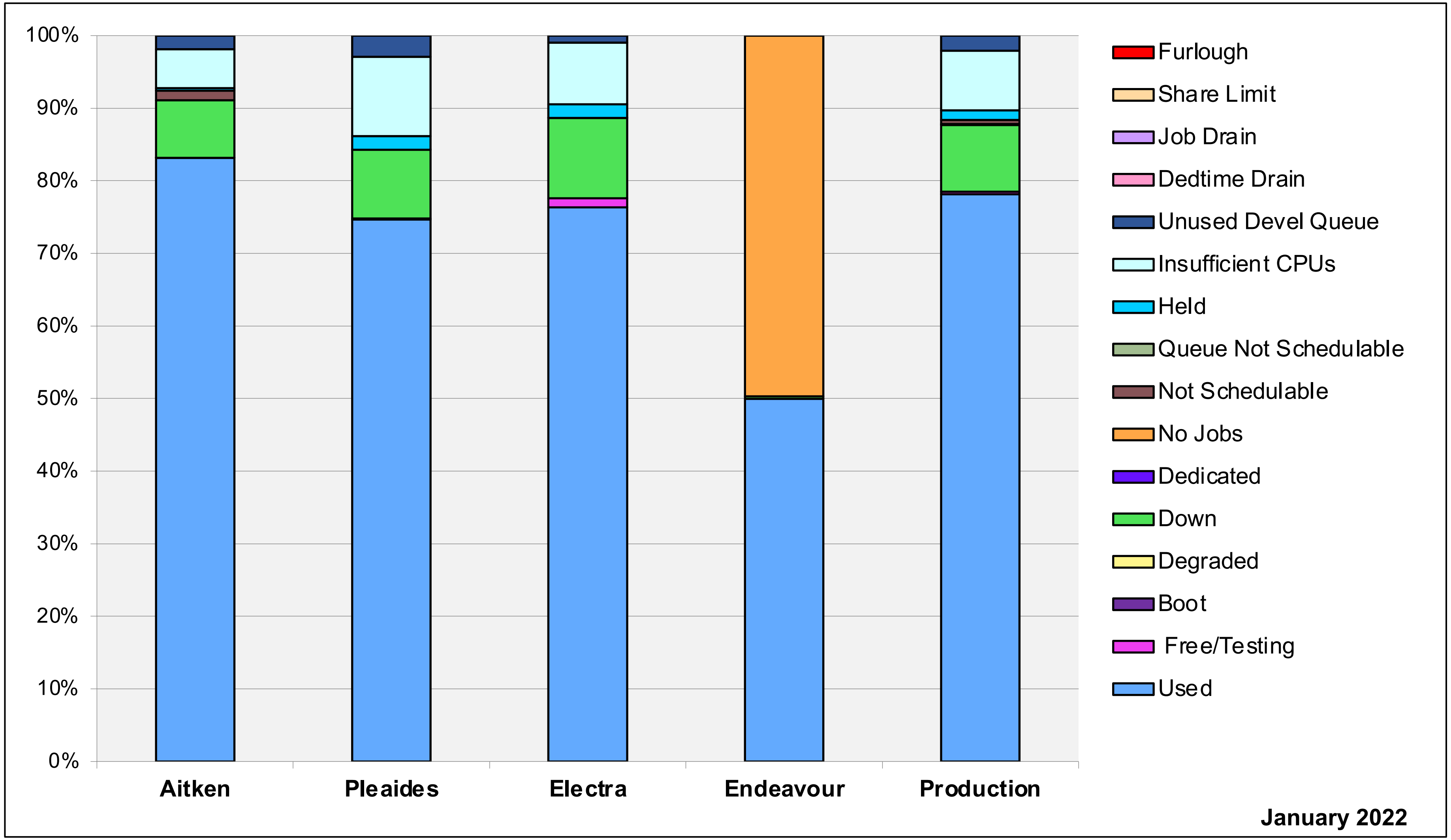
News and Events

- **When Water is Coming from All Sides**, *Texas Advanced Computing Center*, January 13, 2022—Researchers at the National Oceanographic and Atmospheric Administration teamed up with colleagues at the Virginia Institute of Marine Science at William & Mary to develop and test the world's first three-dimensional operational storm surge model. The research was enabled by supercomputers at the NASA Advanced Supercomputing facility and the Texas Advanced Computing Center.
  https://www.tacc.utexas.edu/-/when-water-is-coming-from-all-sides
  - **NOAA, William & Mary Researchers' Team with TACC to Develop First-Ever 3D Compound Inland-Coastal Flooding Guidance System**, *ECO Magazine*, January 17, 2022. *https://www.ecomagazine.com/news/coasts/noaa-william-mary-researchers-team-with-tacc-to-develop-first-ever-3d-compound-inland-coastal-flooding-guidance-system*
- **Helping to Improve Launch Safety**, *This Week @ NASA*, January 7, 2022—The first "This Week @ NASA" video of the year went on location with the Electra supercomputer and featured a simulation by NAS Division researchers. The simulation helps engineers understand how vibration levels during various launch abort scenarios might affect the Orion spacecraft's launch abort system.
  https://www.nasa.gov/sites/default/files/atoms/video/nhq_2022_0107_twn.mp4

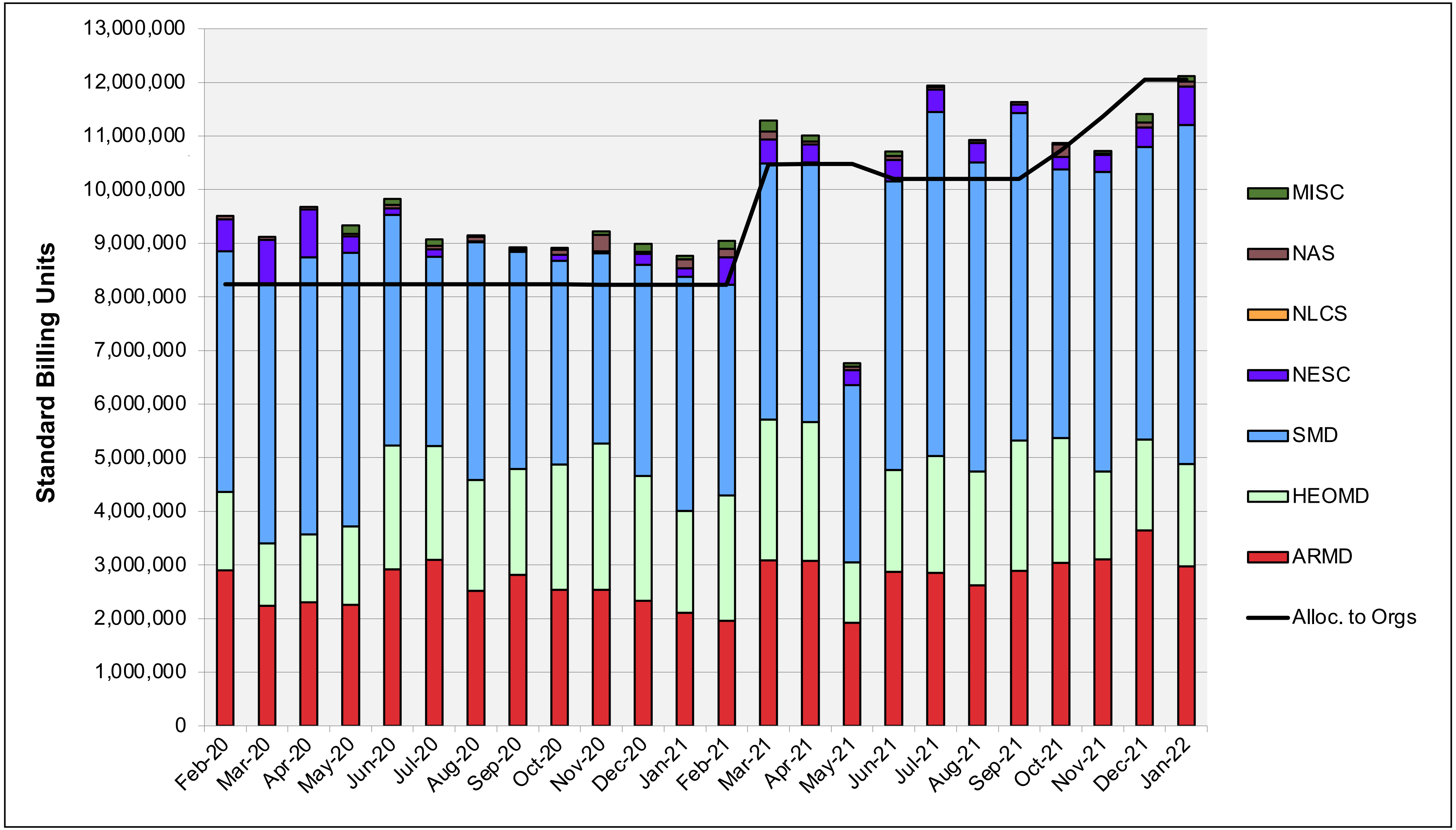
News and Events: Social Media

- **Coverage of NAS Stories**
  - NAS hyperwall social media feature:
    - NASA Ames: Facebook 84 likes, 11 comments, 25 shares; Twitter 8 retweets, 5 quote tweets, 96 likes.
    - NASA Supercomputing: Facebook 724 users reached, 22 engagements, 12 likes, 4 shares; Twitter 9 retweets, 1 quote tweet, 17 likes.
  - NASA Day of Remembrance Campaign:
    - NAS: Twitter 14 retweets, 1 quote tweet, 57 likes.

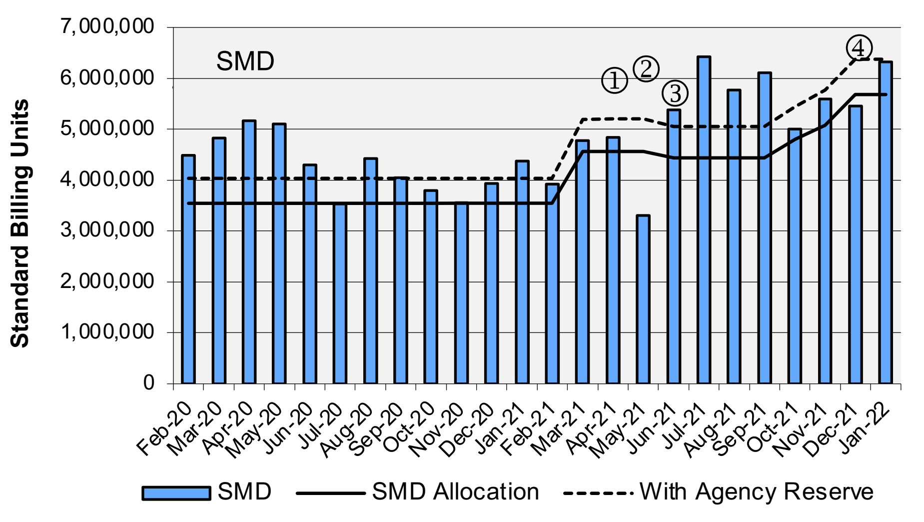
HECC Utilization

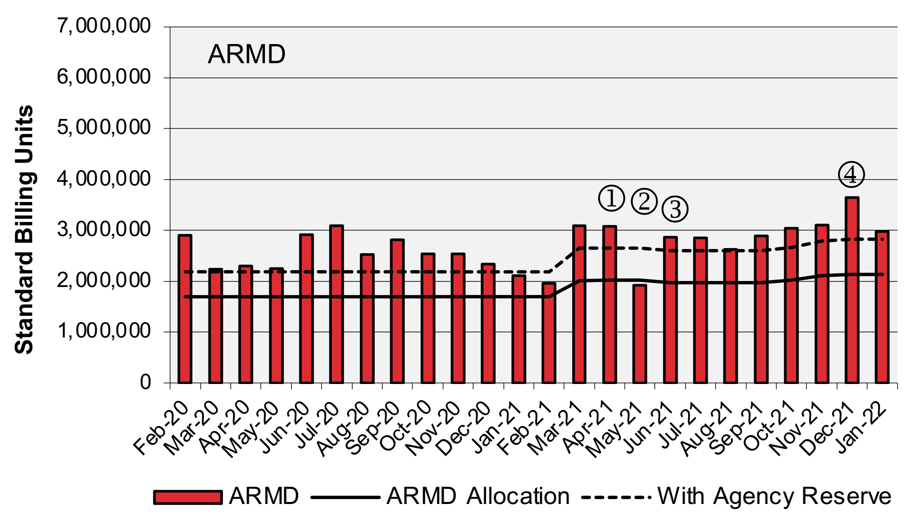


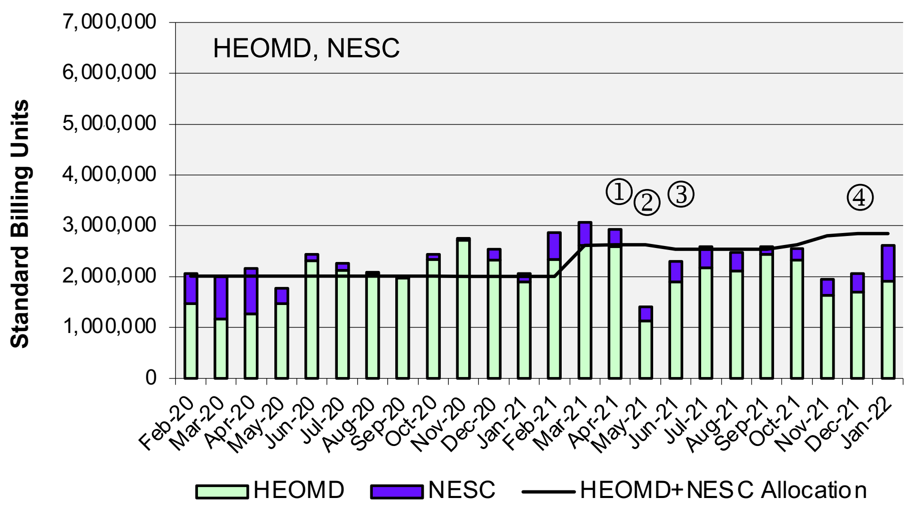
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month







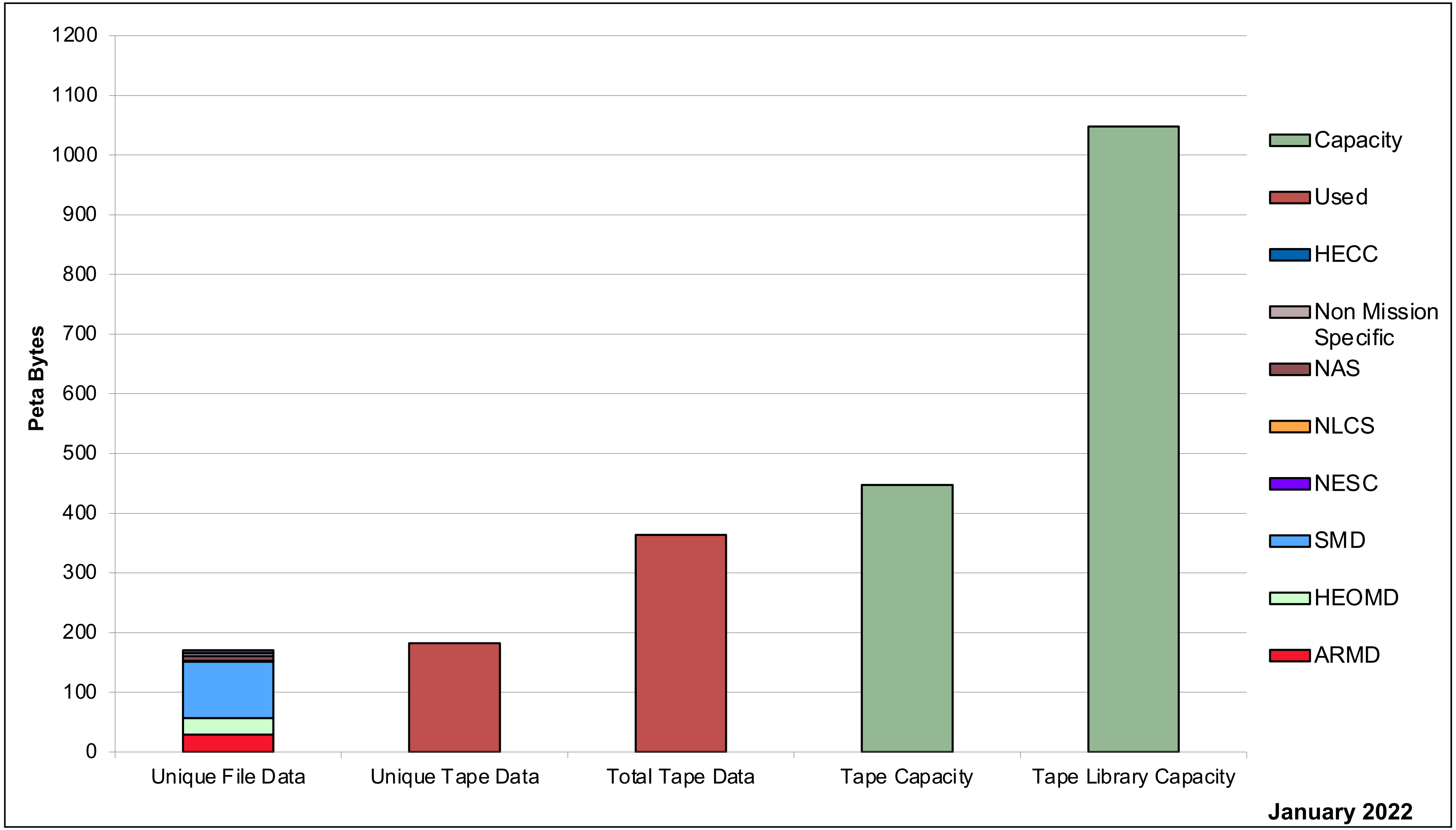
① 8 Rome Apollo racks introduced into Aitken

② Endeavour replaced with new hardware

③ Merope retired

④ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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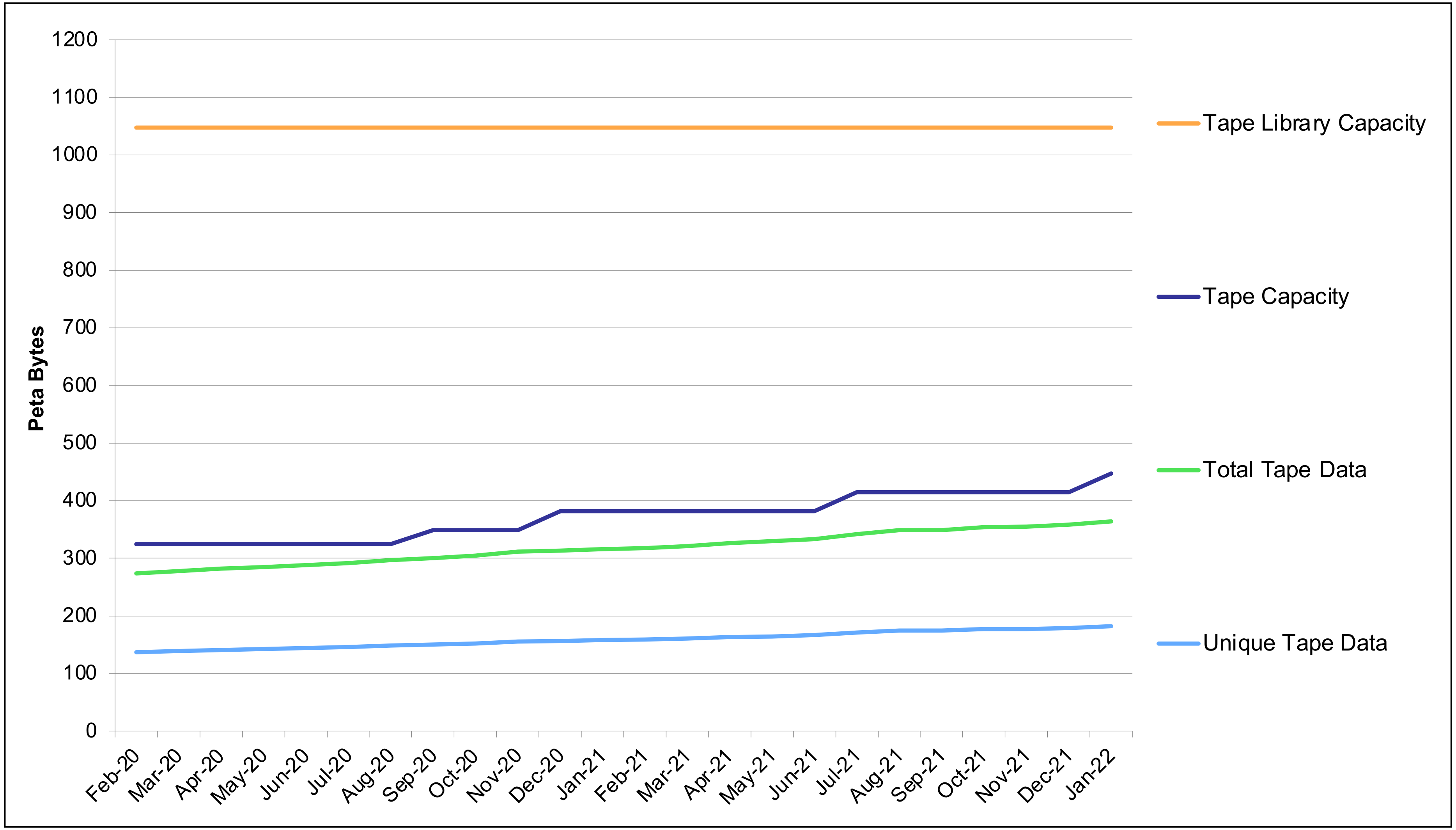
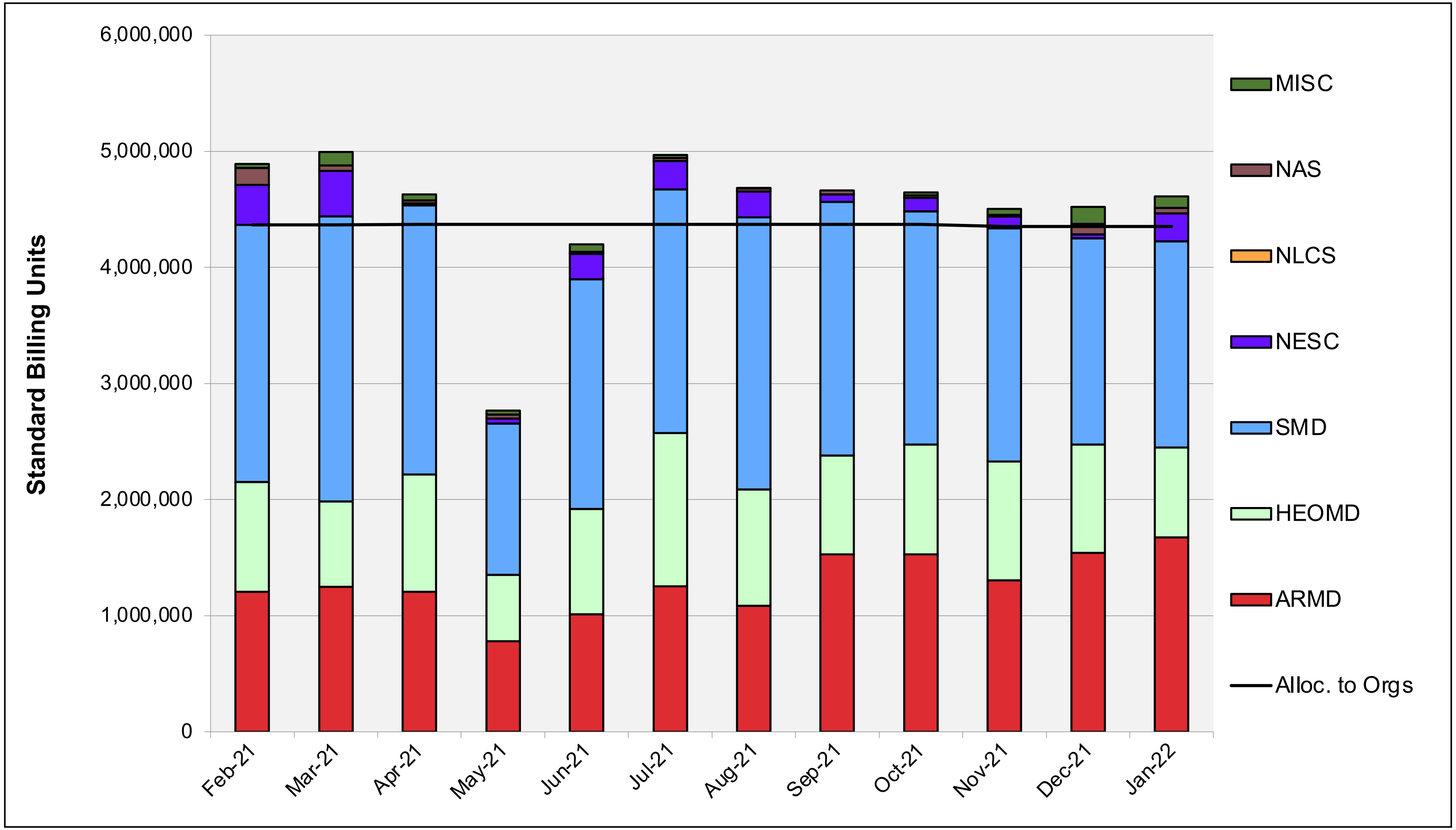
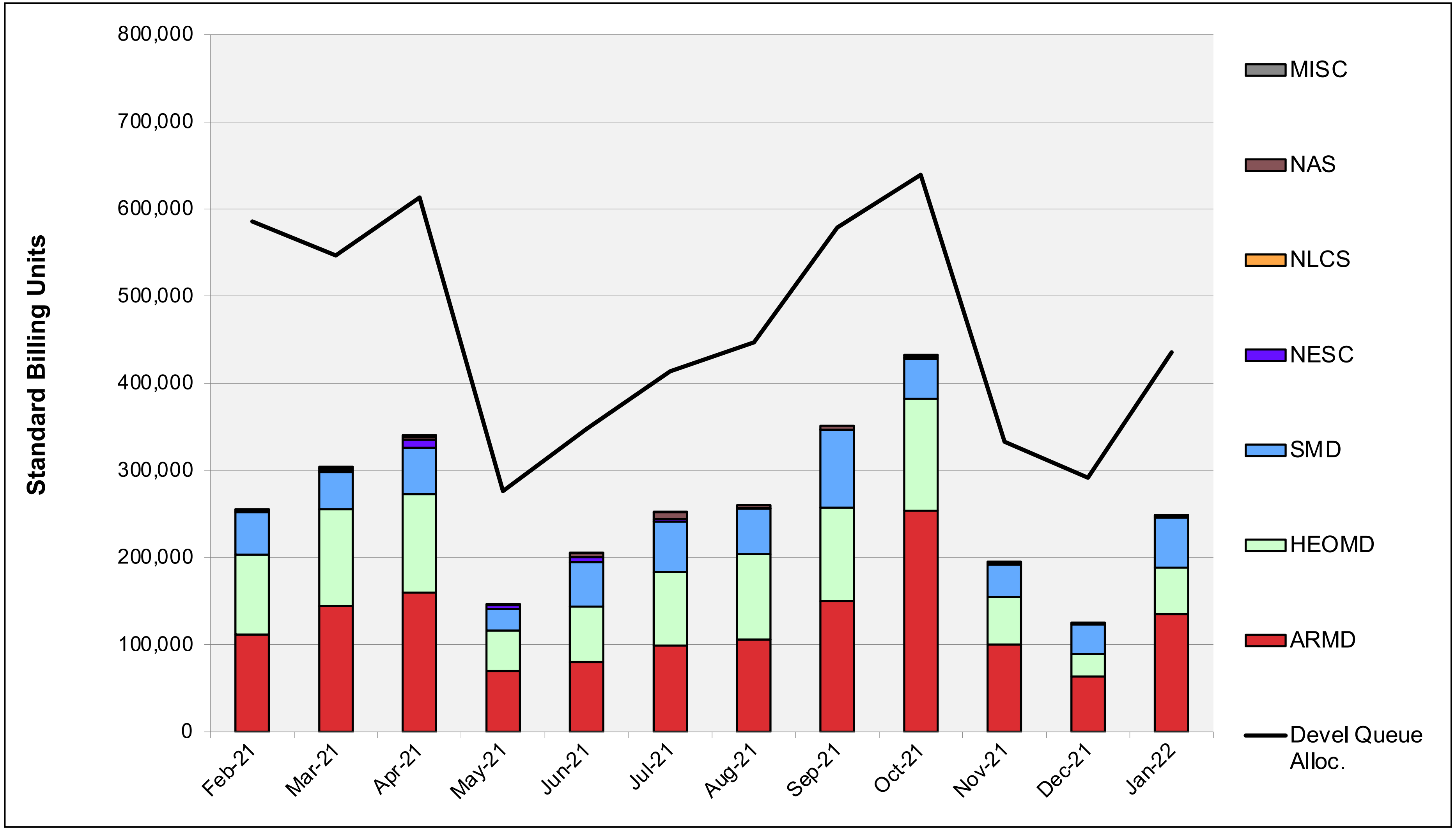


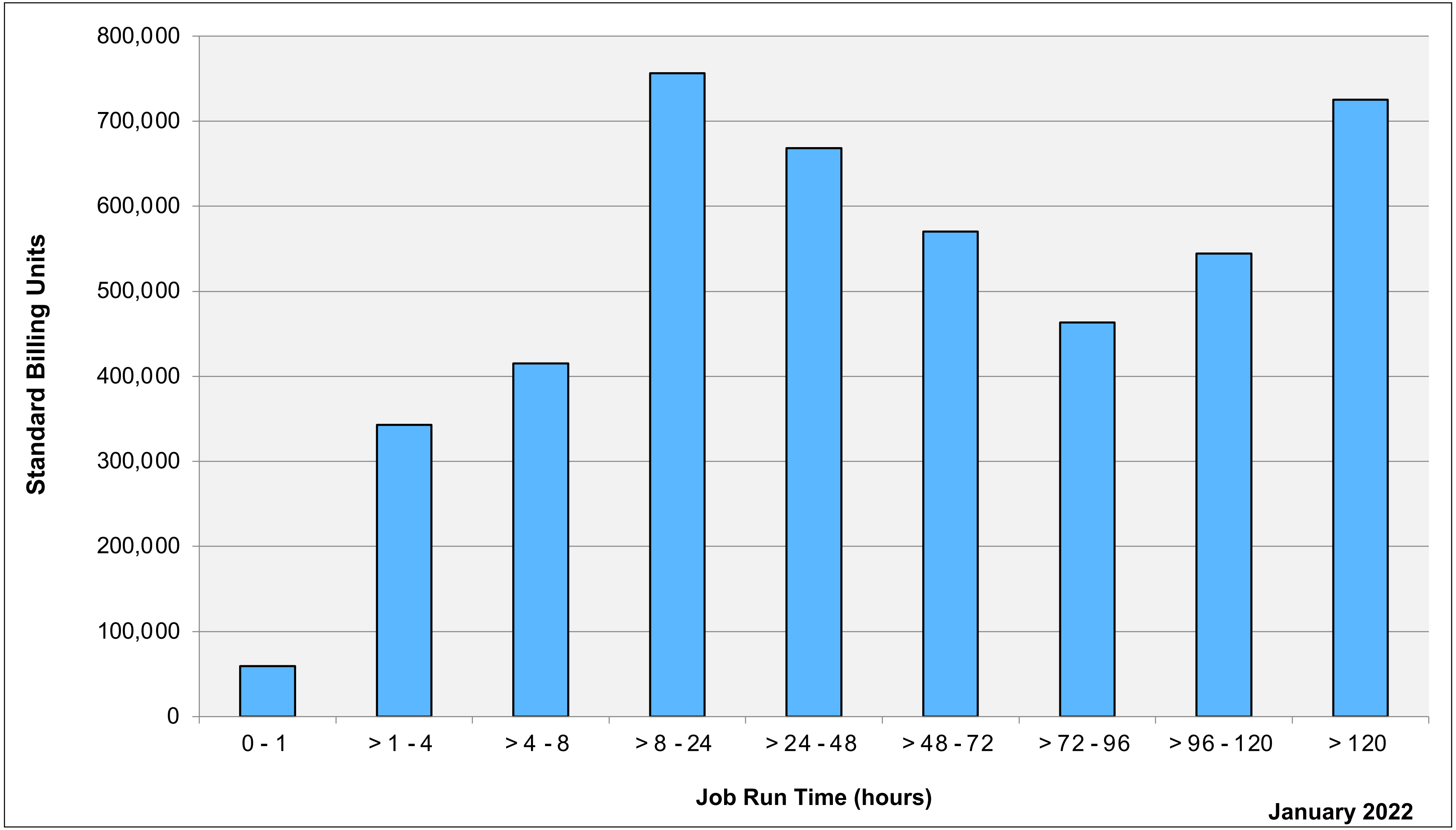
Pleiades: SBUs Reported, Normalized to 30-Day Month



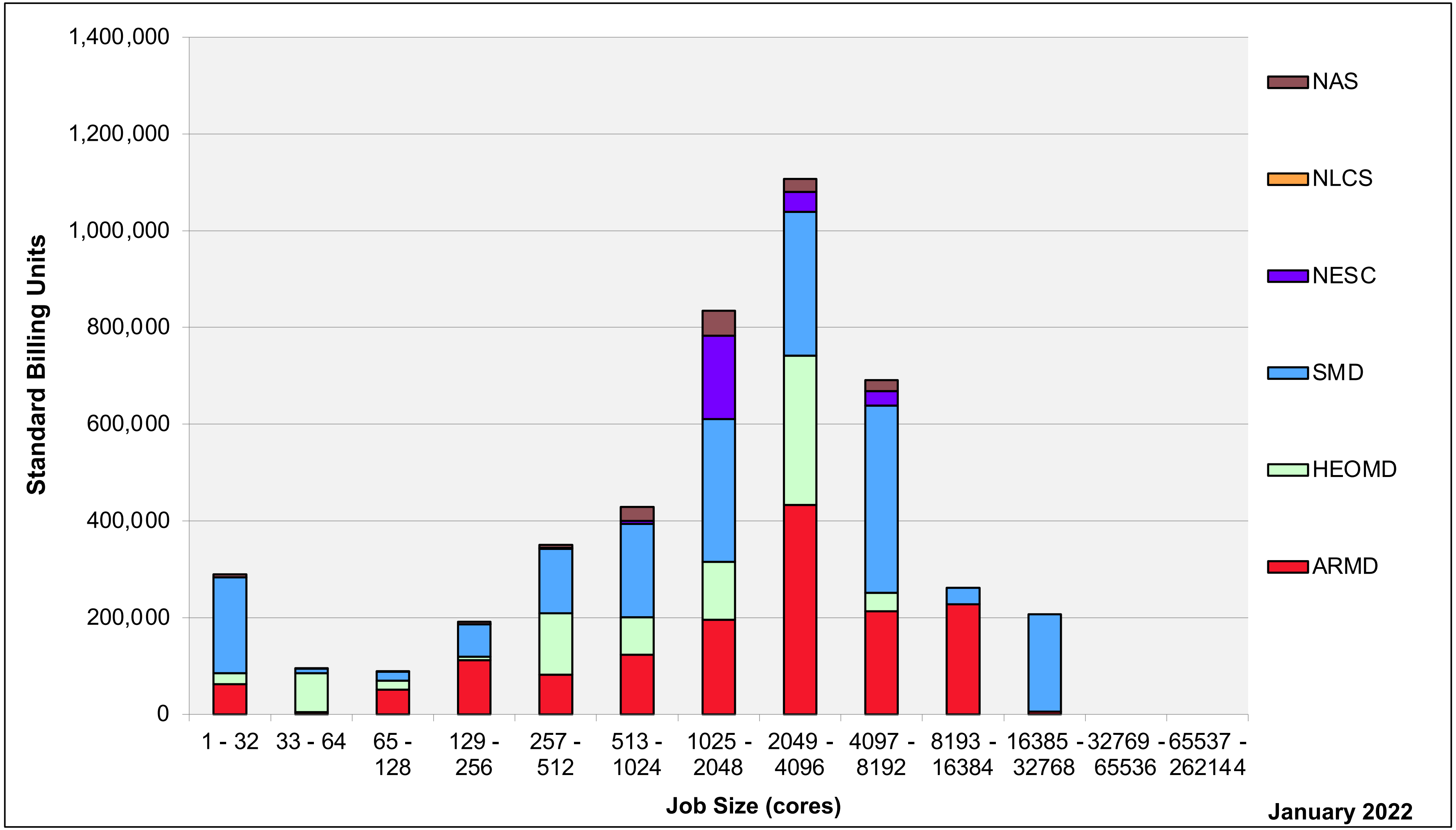
Pleiades: Devel Queue Utilization



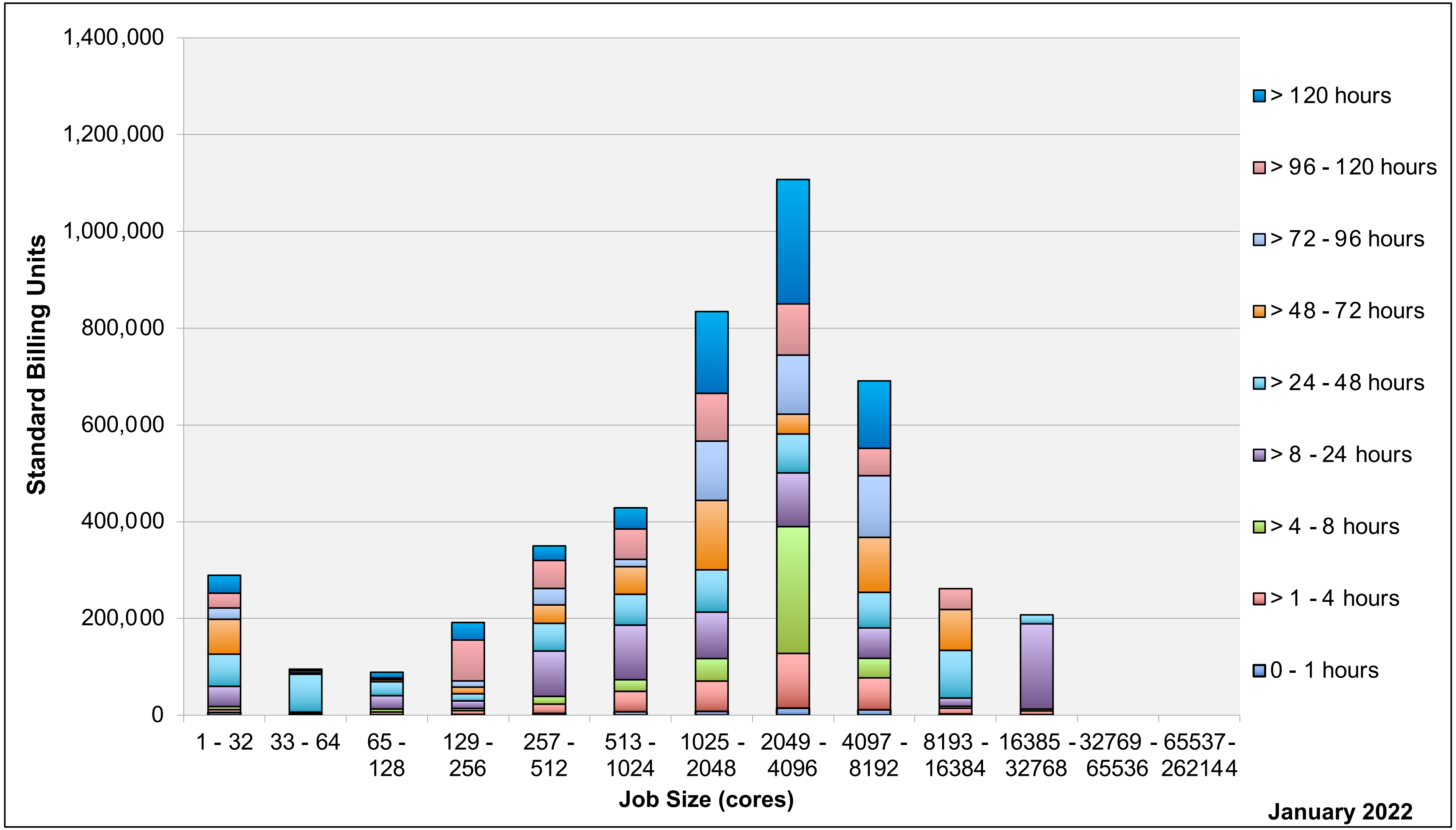
Pleiades: Monthly Utilization by Job Length



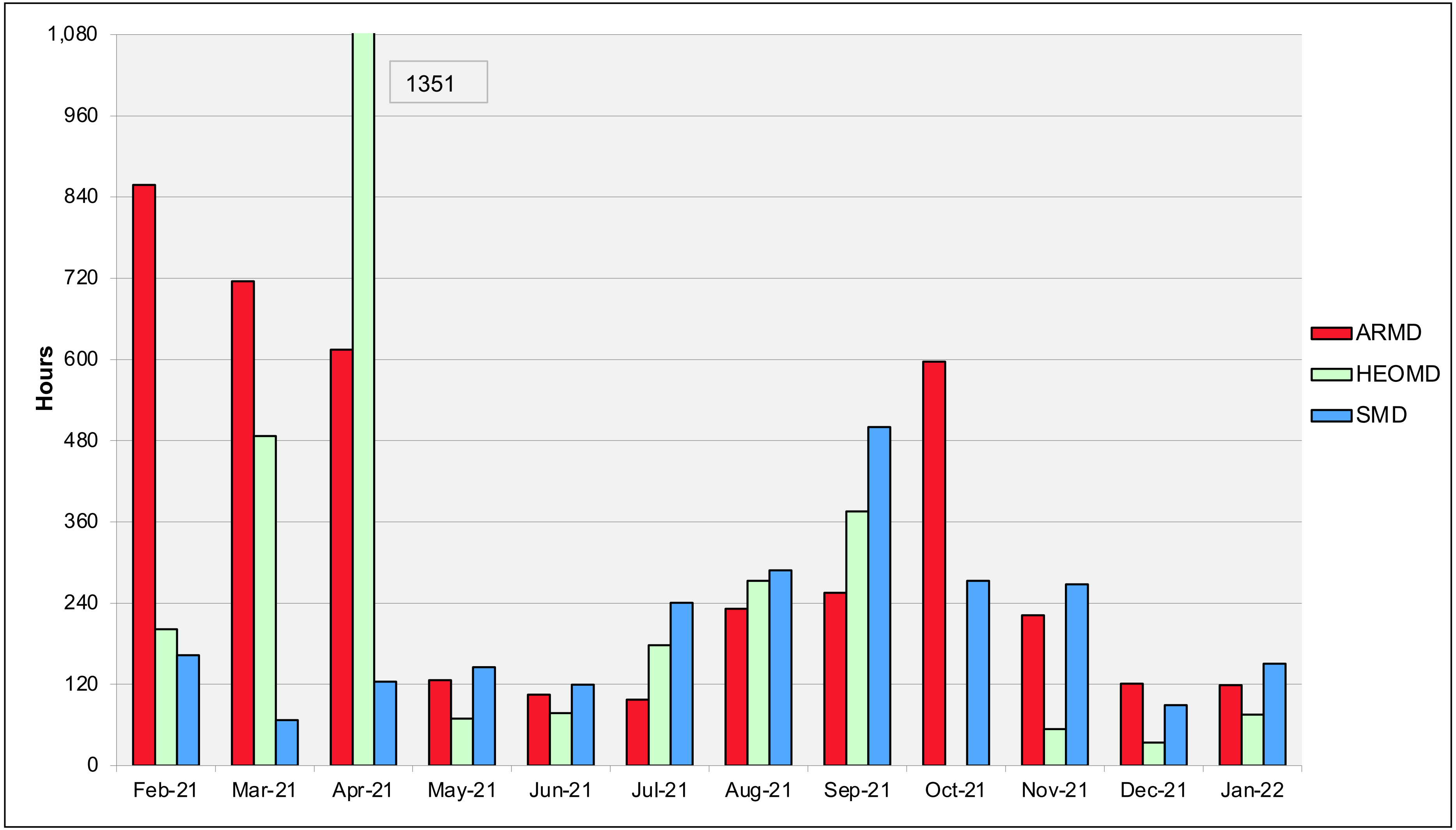
Pleiades: Monthly Utilization by Job Size



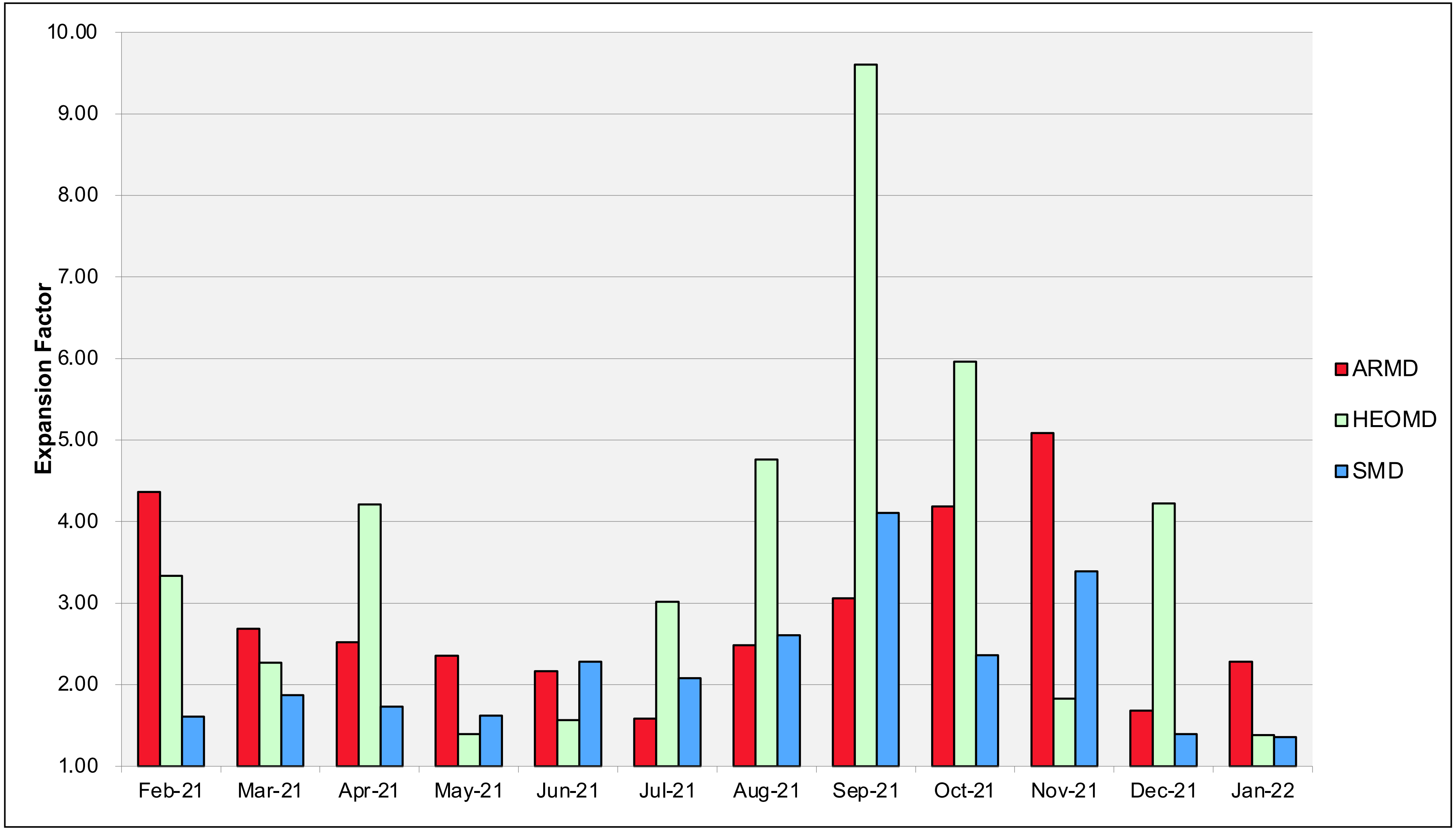
Pleiades: Monthly Utilization by Size and Length



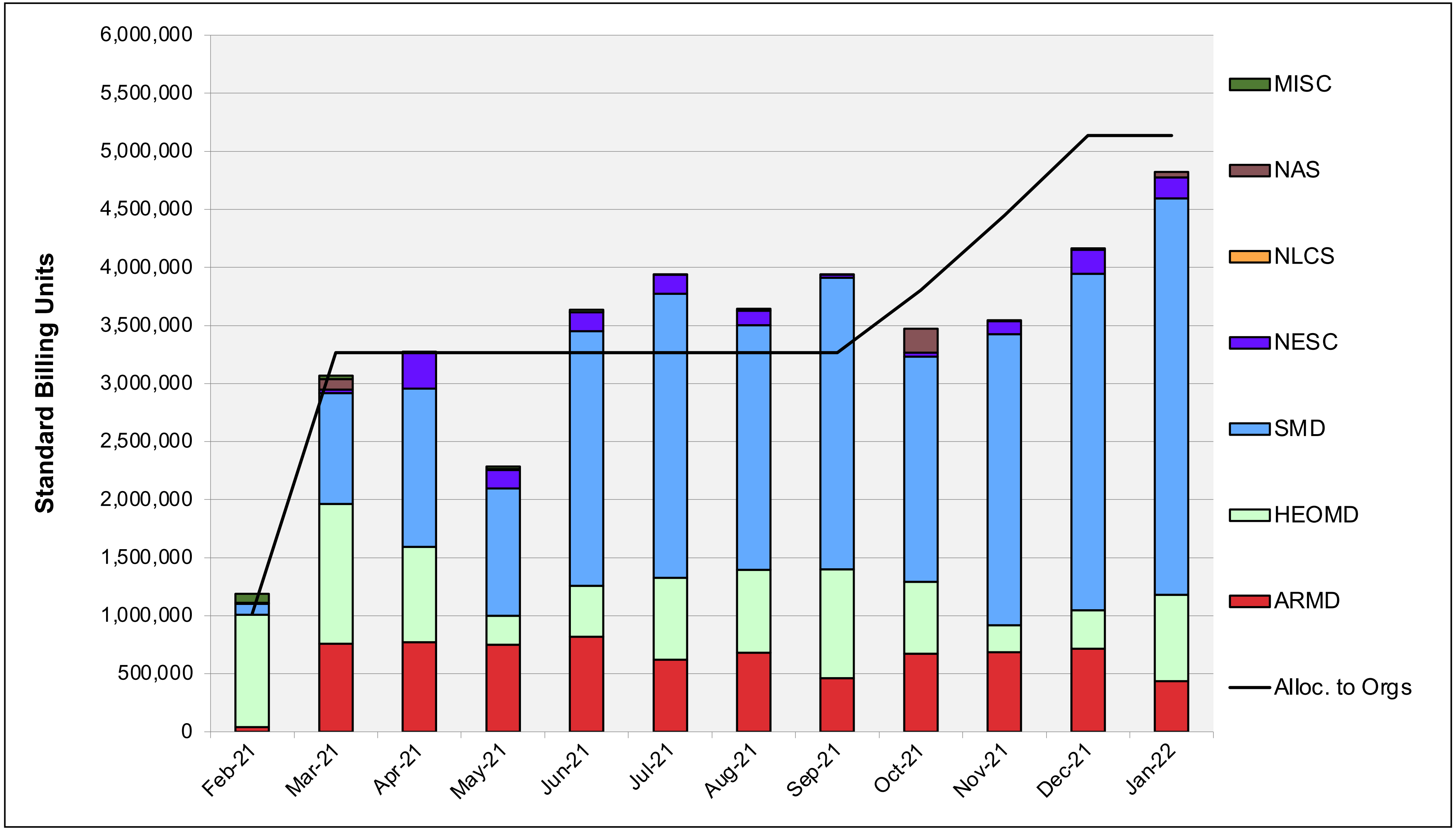
Pleiades: Average Time to Clear All Jobs



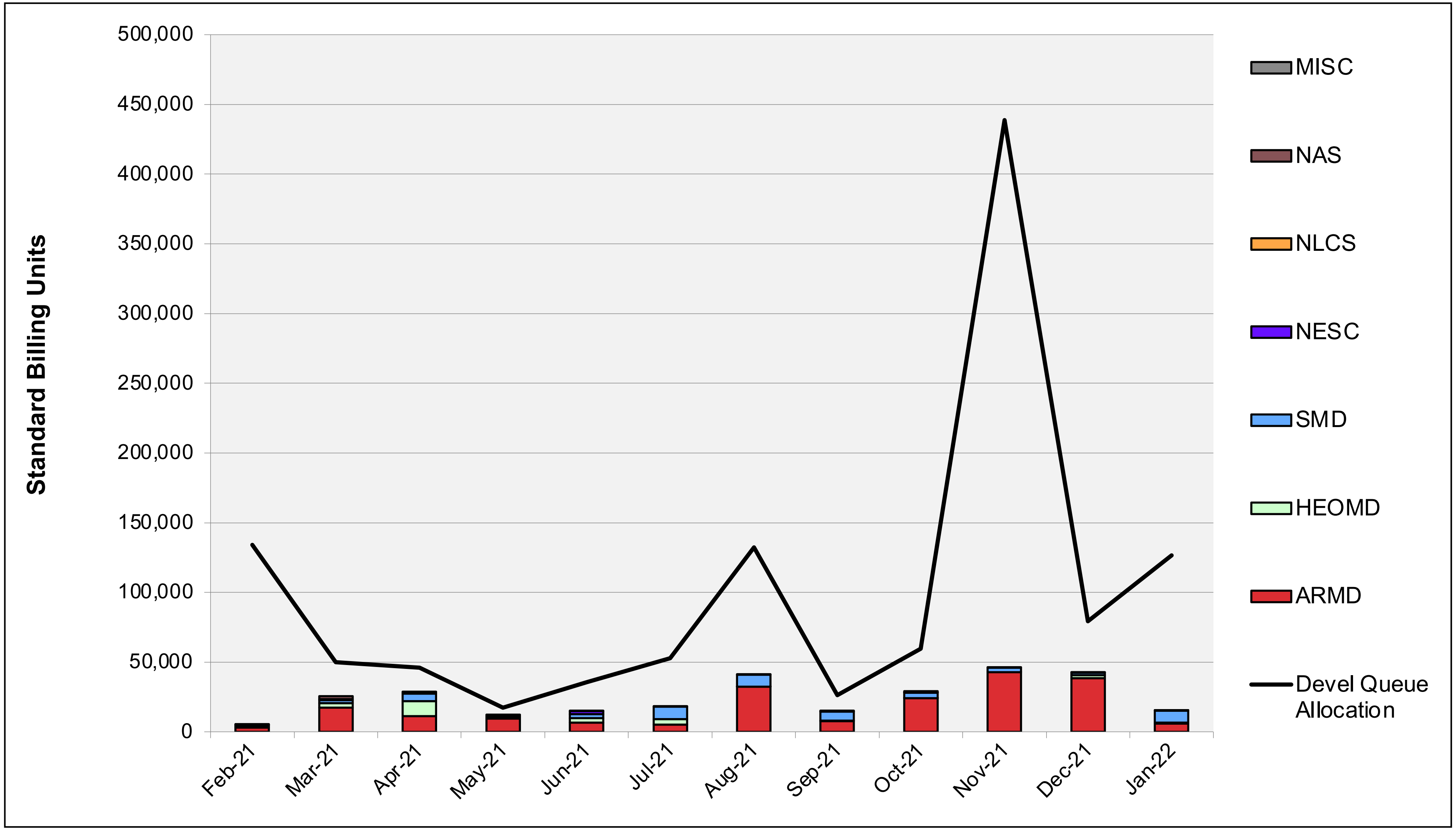
Pleiades: Average Expansion Factor



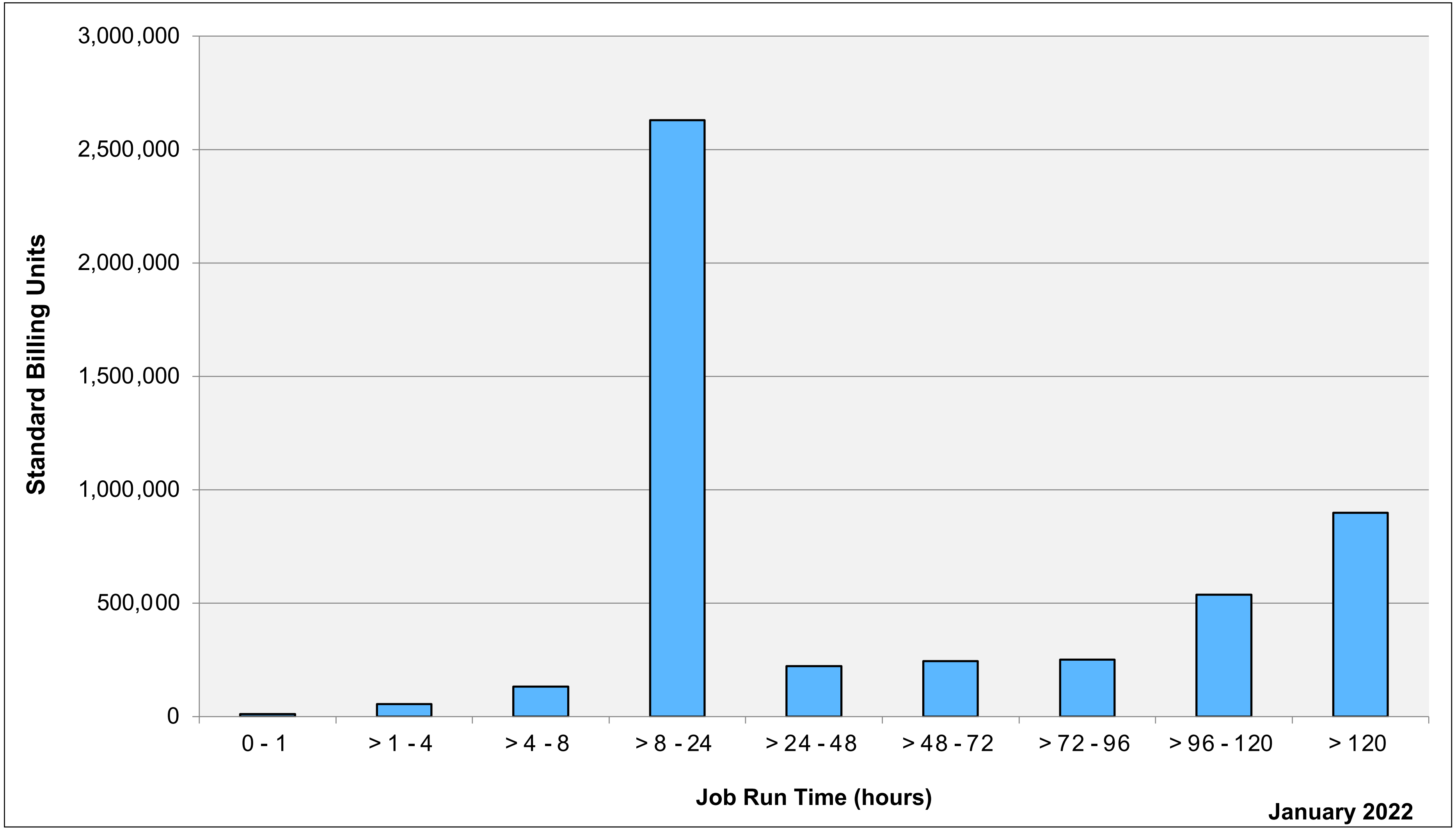
Aitken: SBUs Reported, Normalized to 30-Day Month



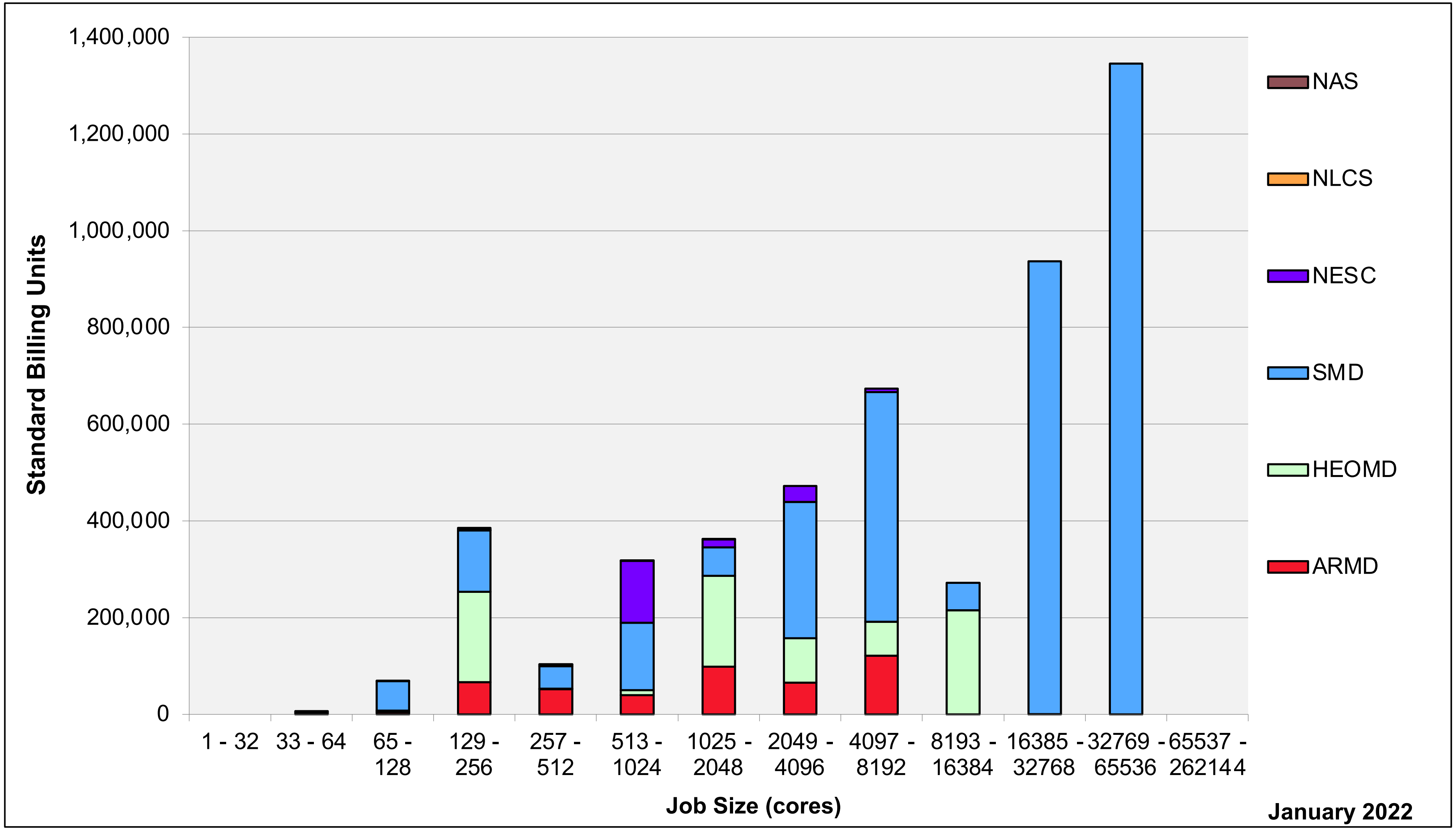
Aitken: Devel Queue Utilization



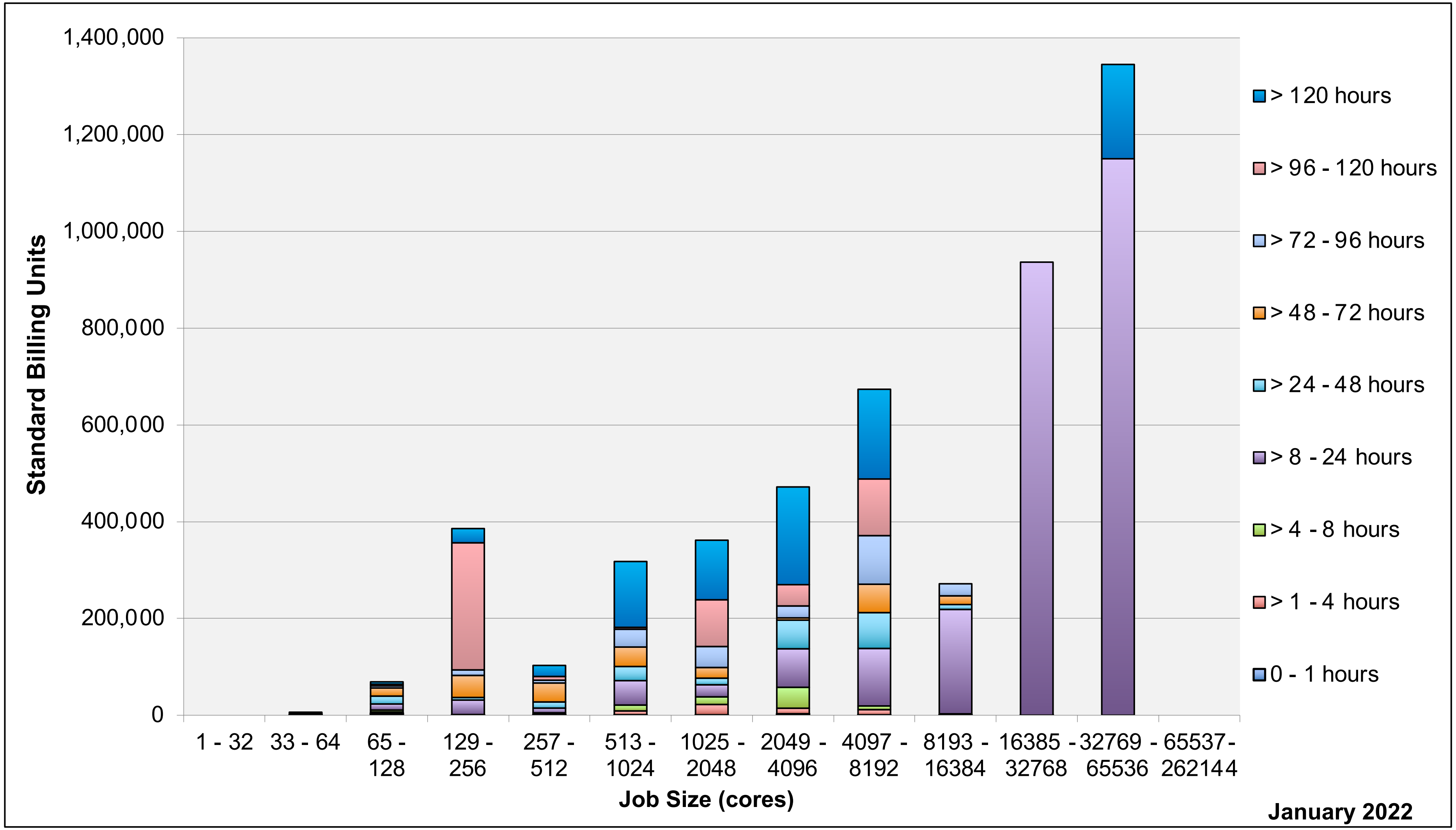
Aitken: Monthly Utilization by Job Length



Aitken: Monthly Utilization by Job Size



Aitken: Monthly Utilization by Size and Length



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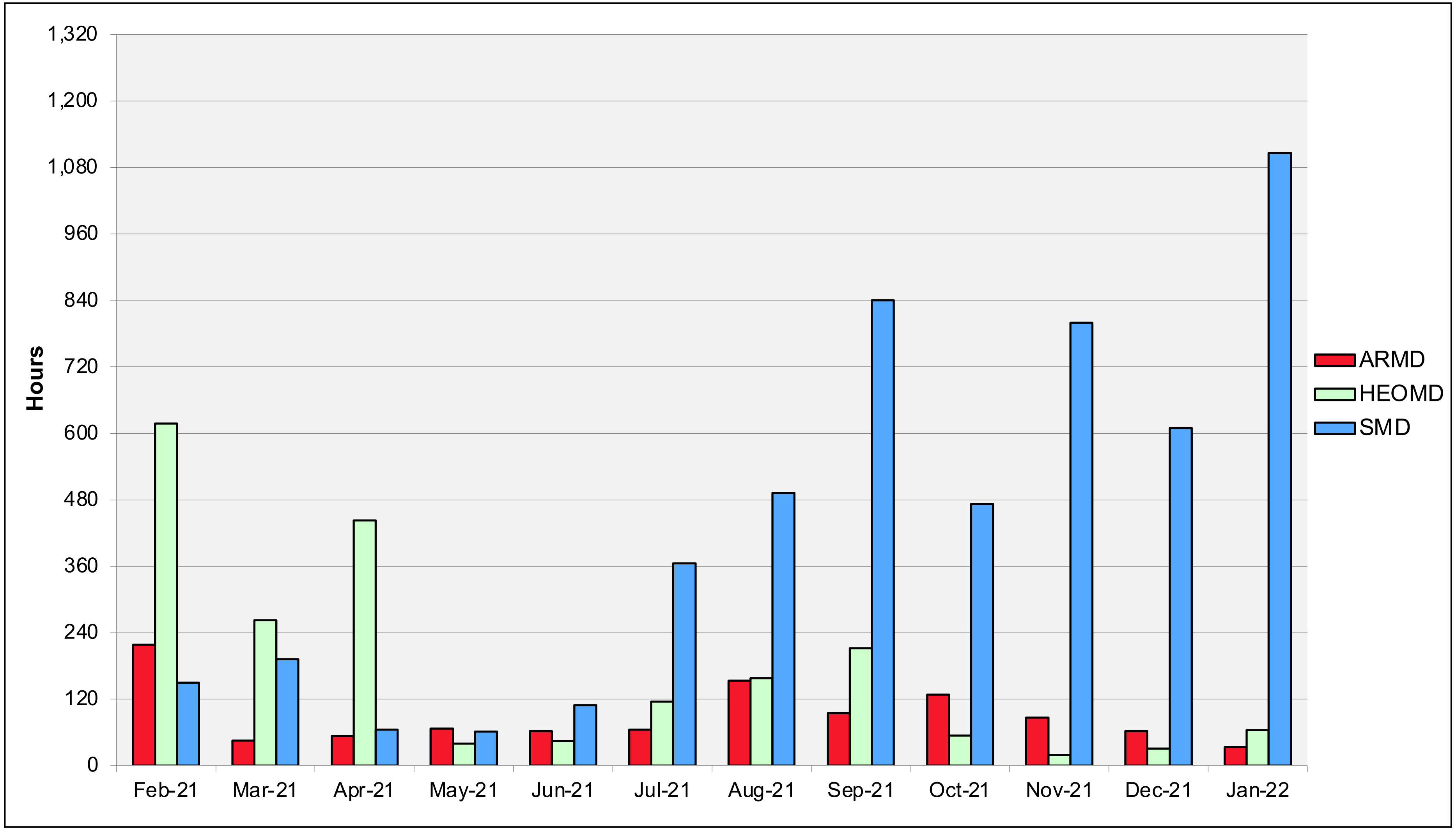
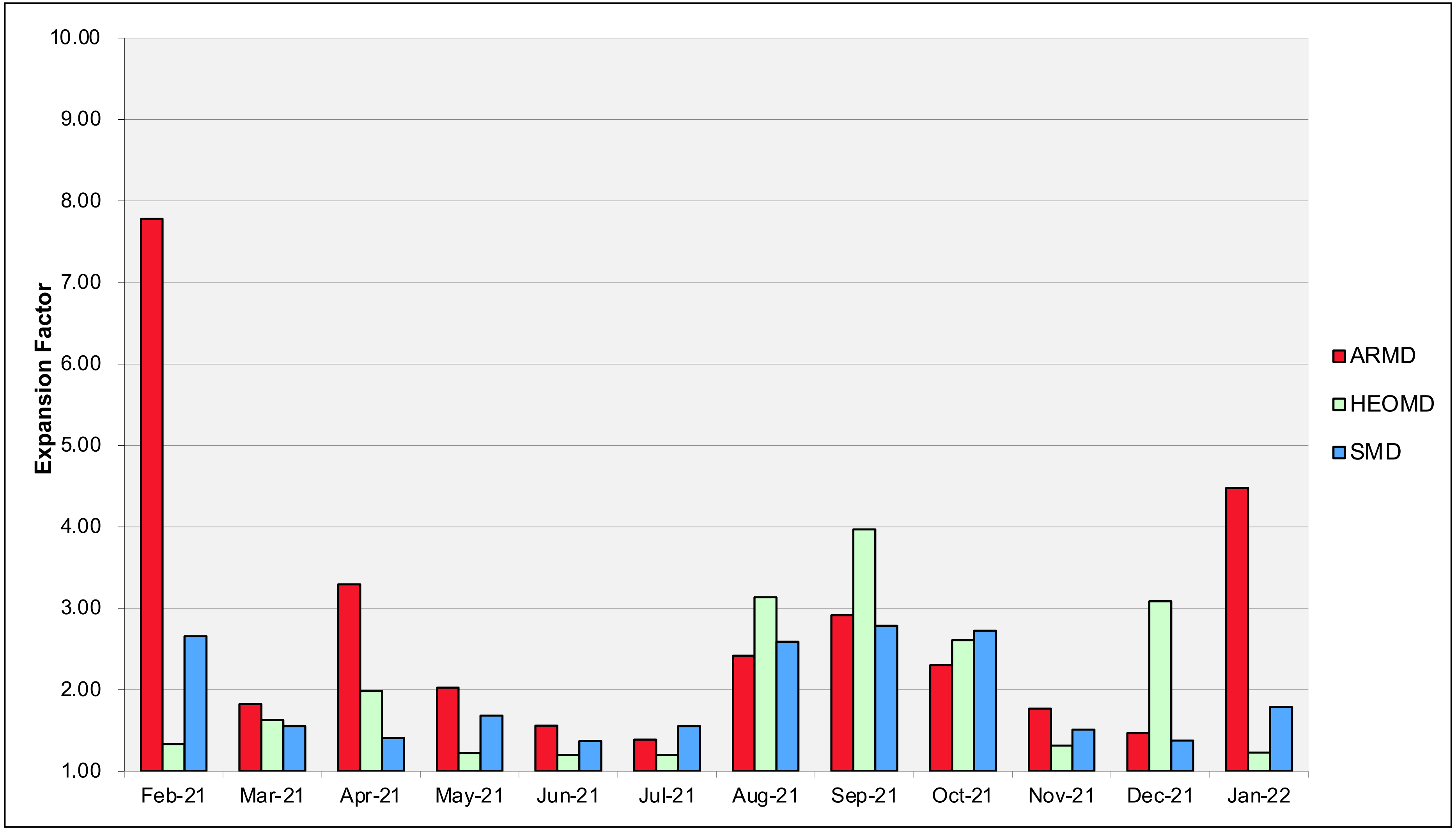
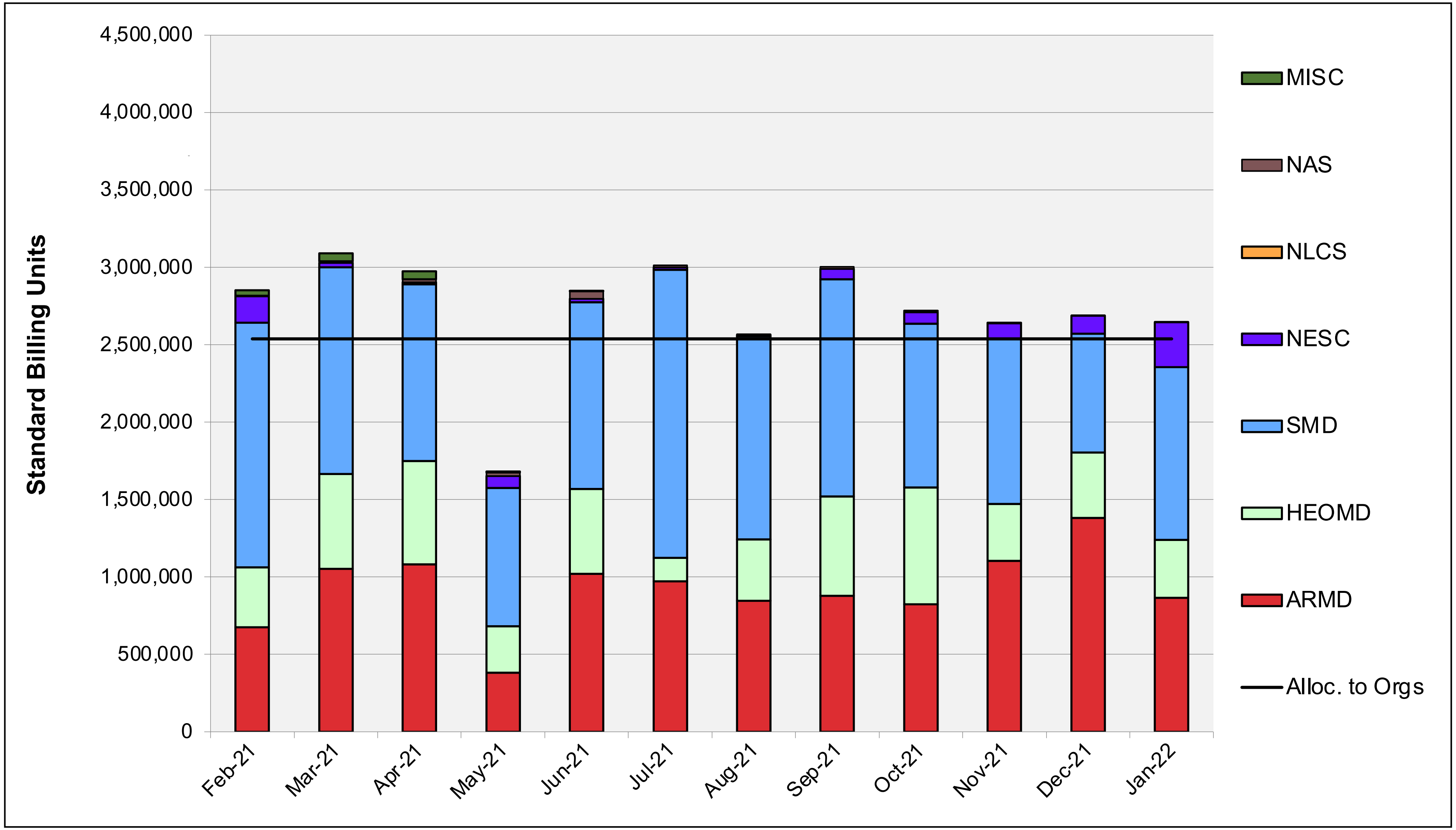


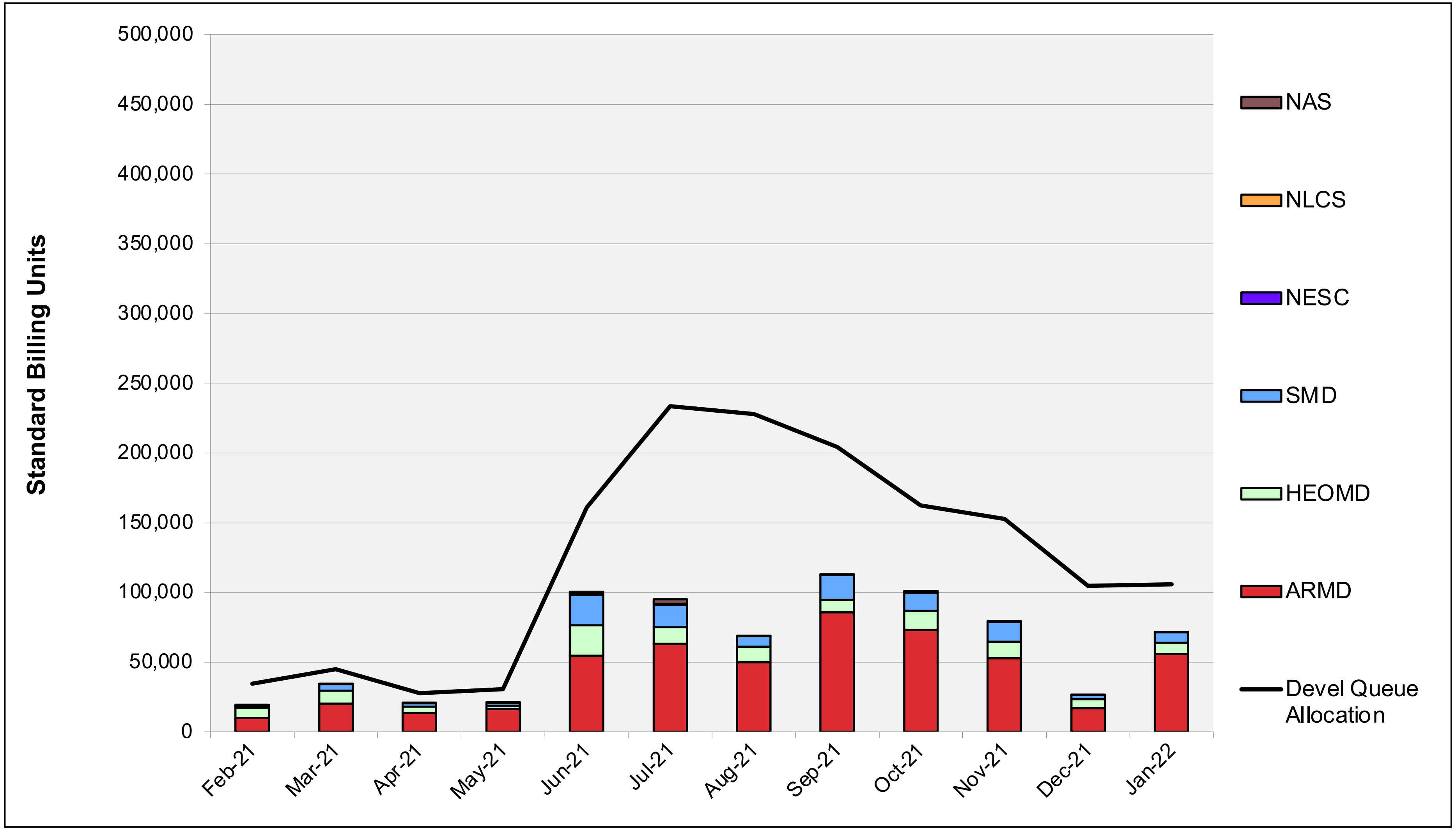
Aitken: Average Expansion Factor



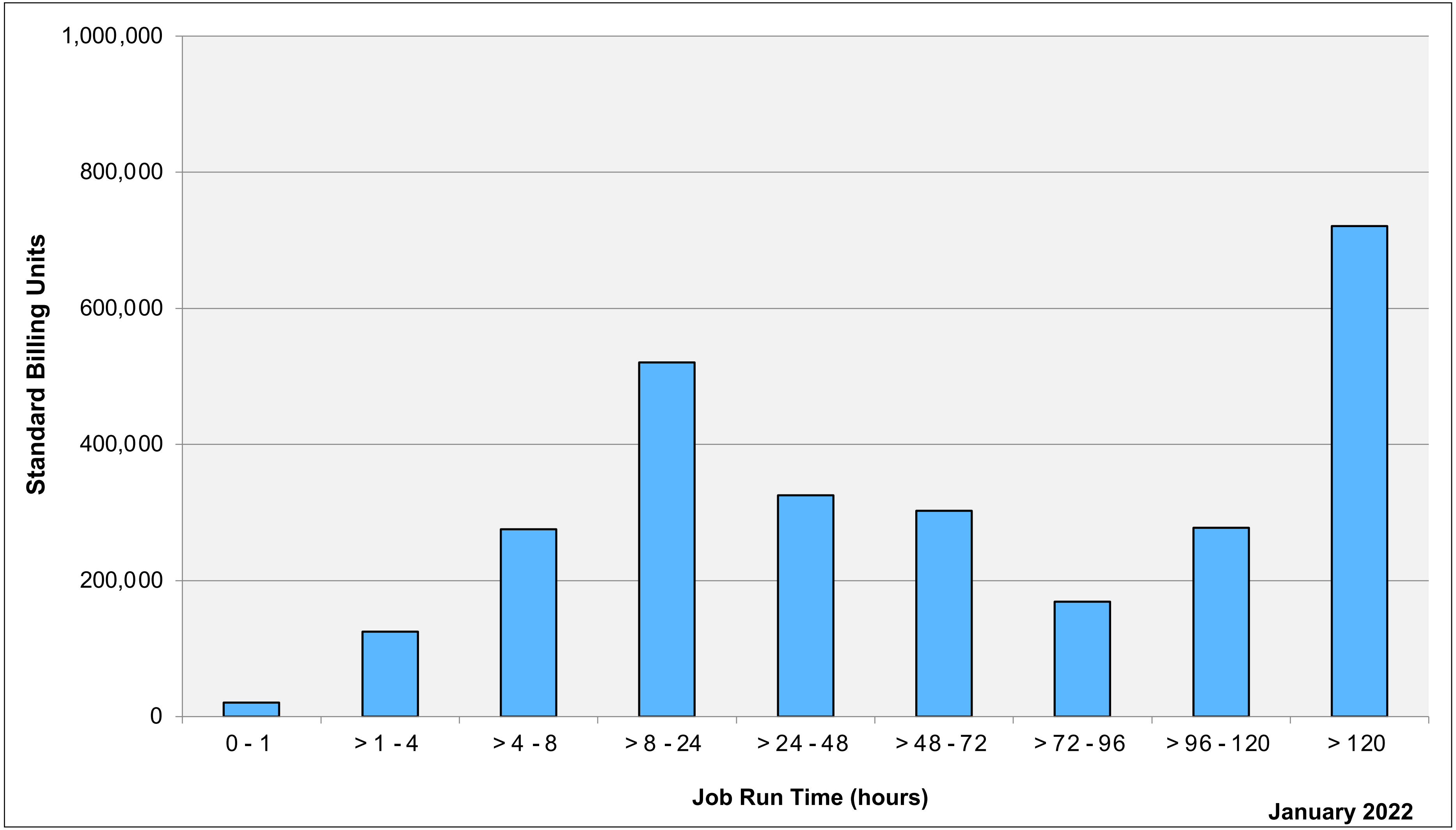
Electra: SBUs Reported, Normalized to 30-Day Month



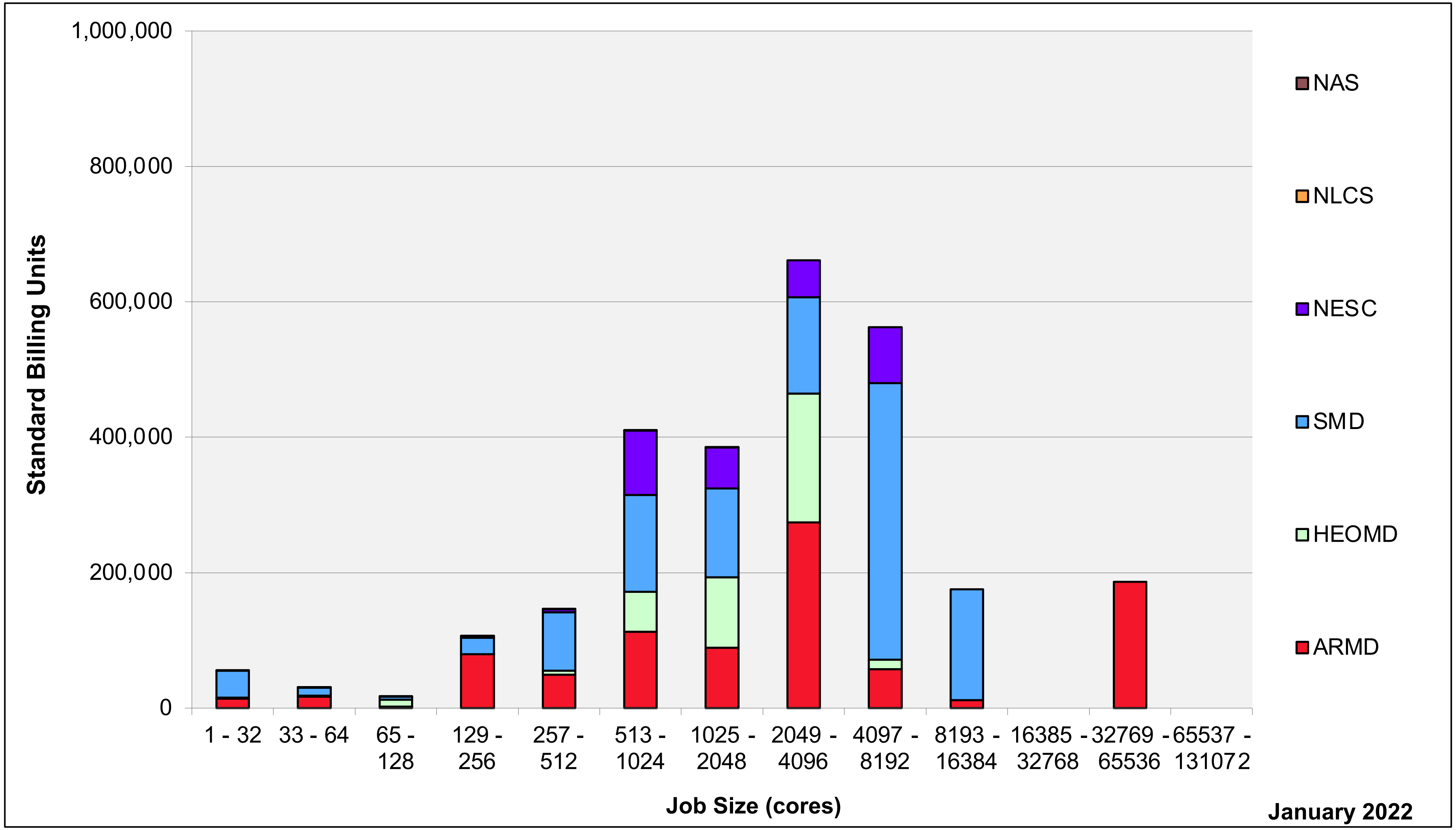
Electra: Devel Queue Utilization



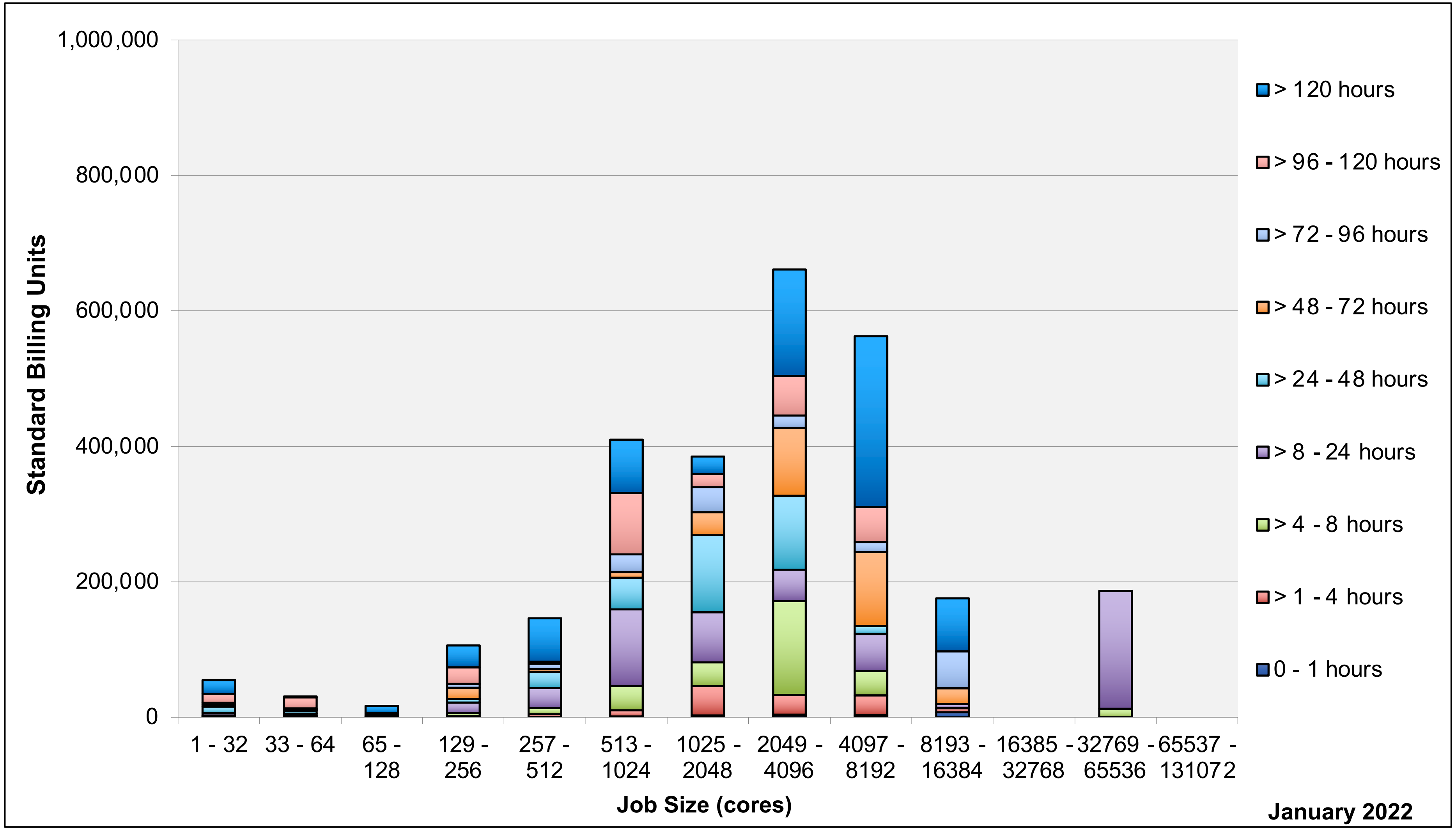
Electra: Monthly Utilization by Job Length



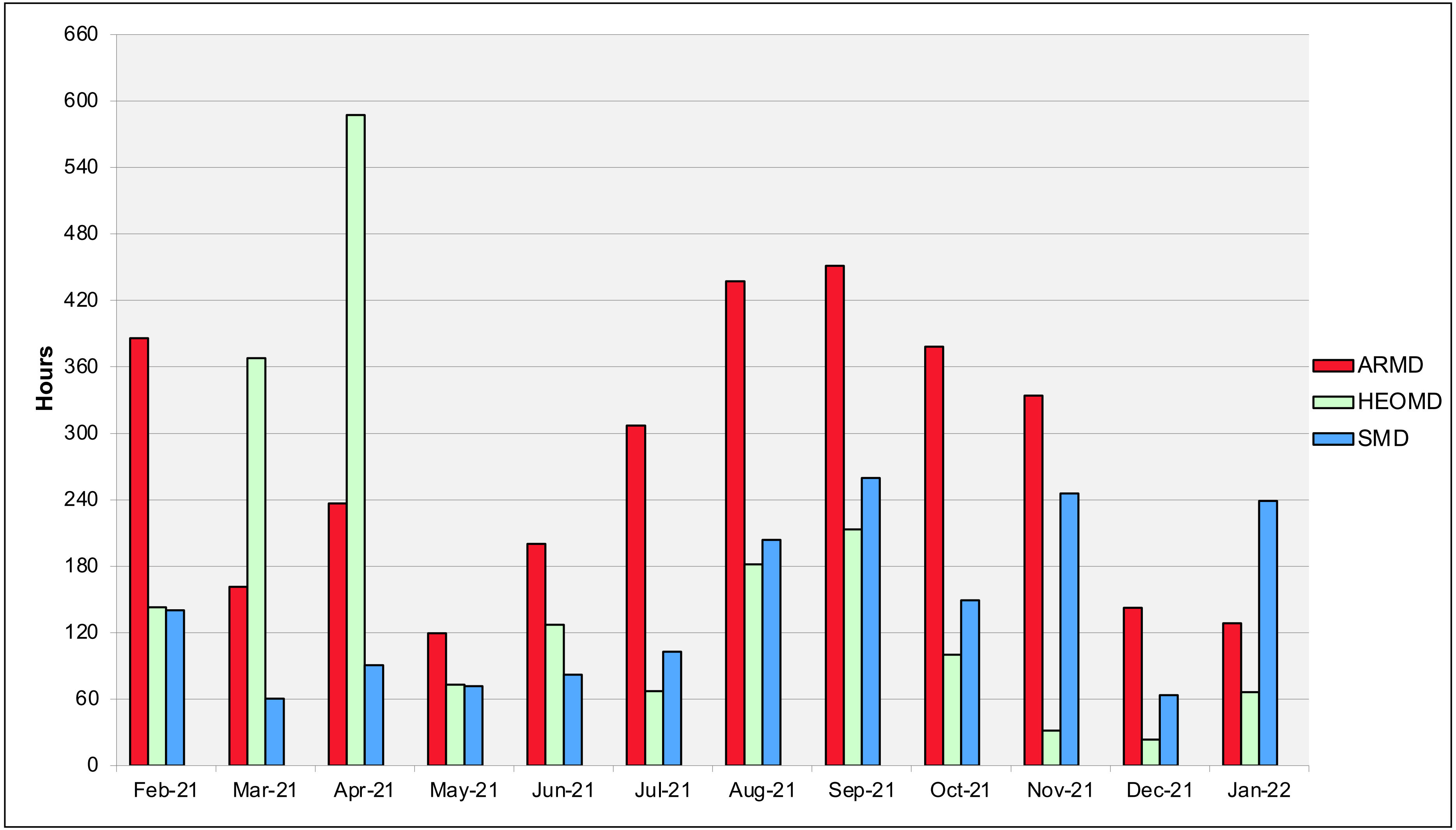
Electra: Monthly Utilization by Job Size



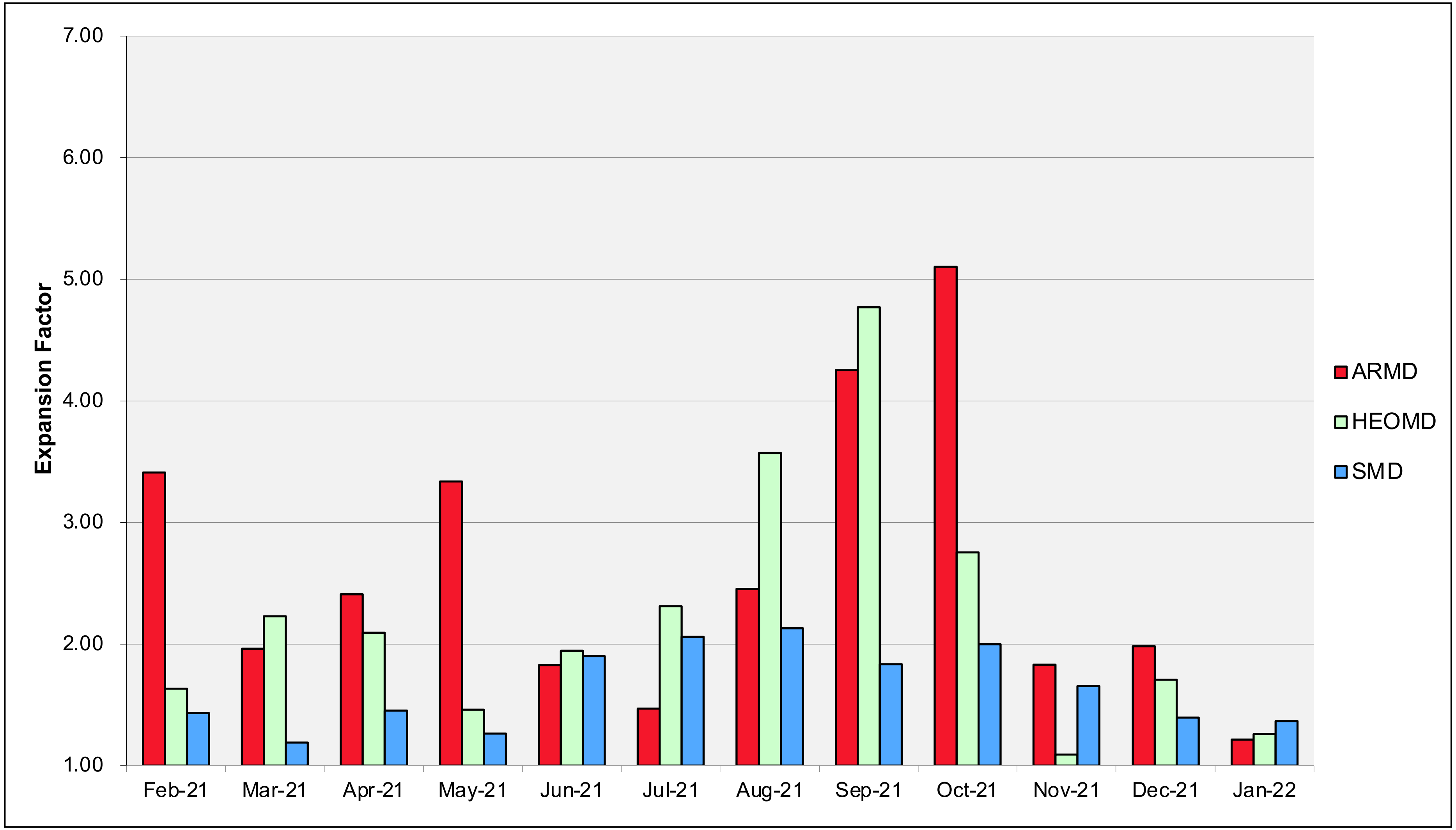
Electra: Monthly Utilization by Size and Length



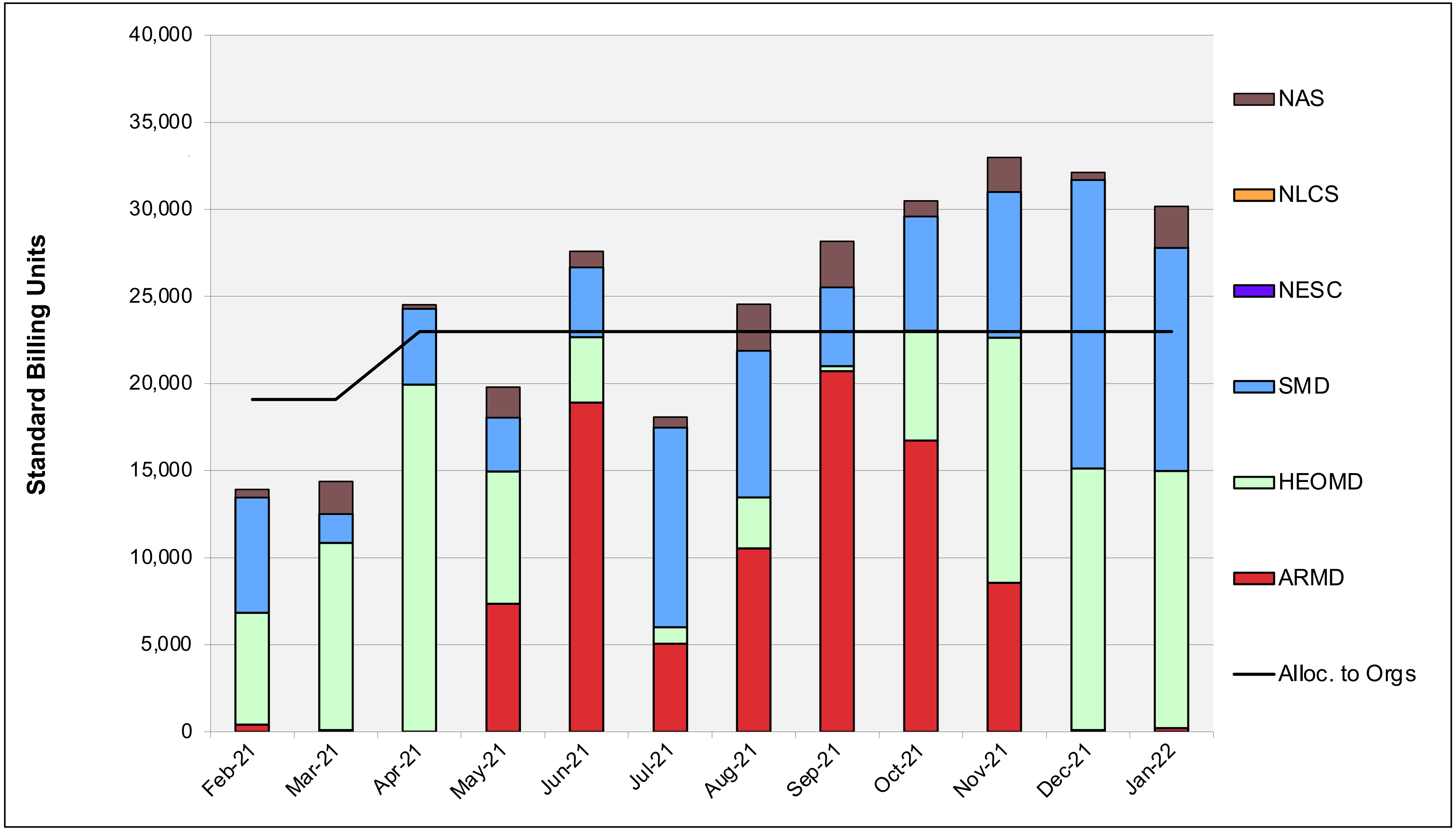
Electra: Average Time to Clear All Jobs



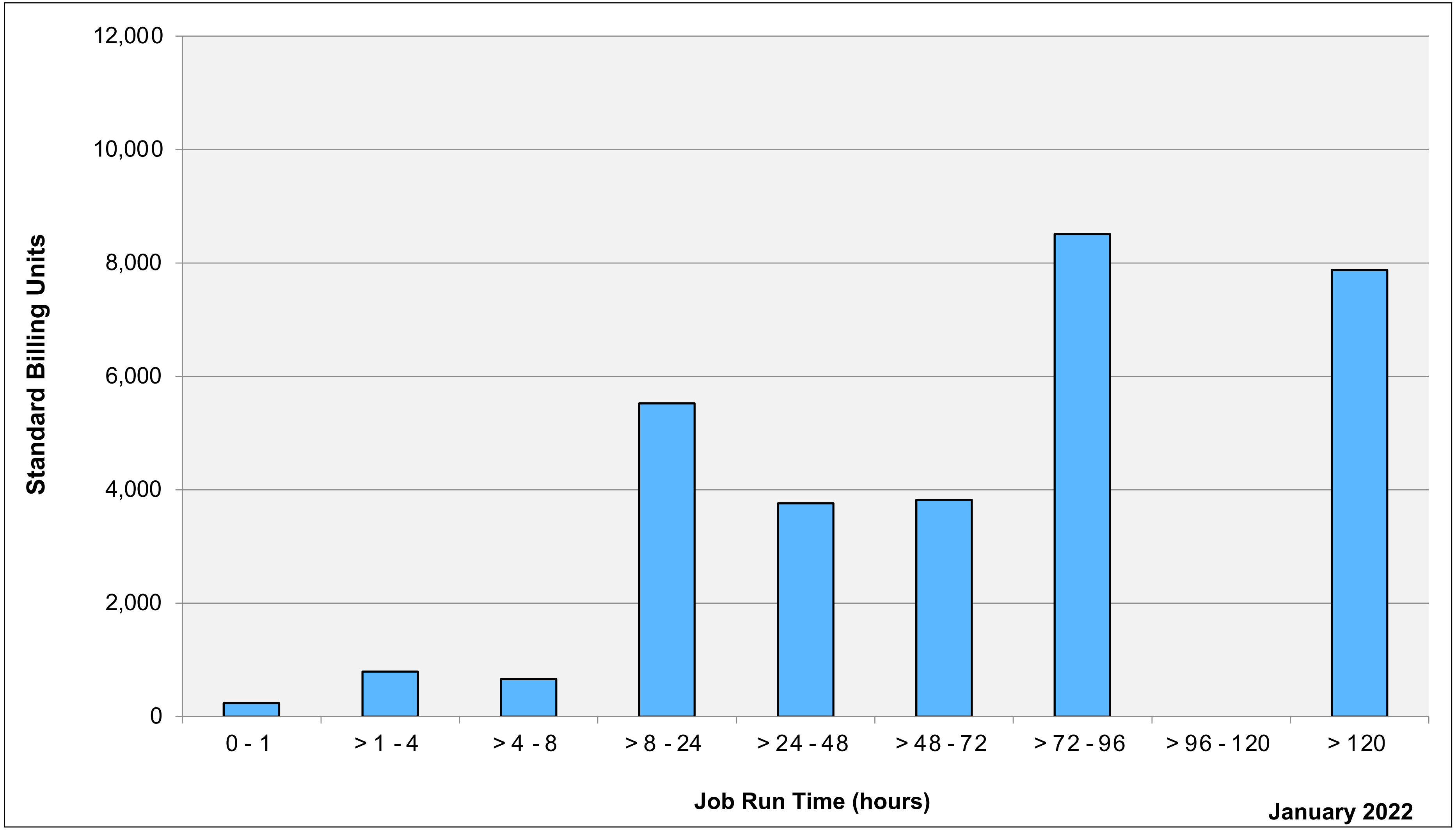
Electra: Average Expansion Factor



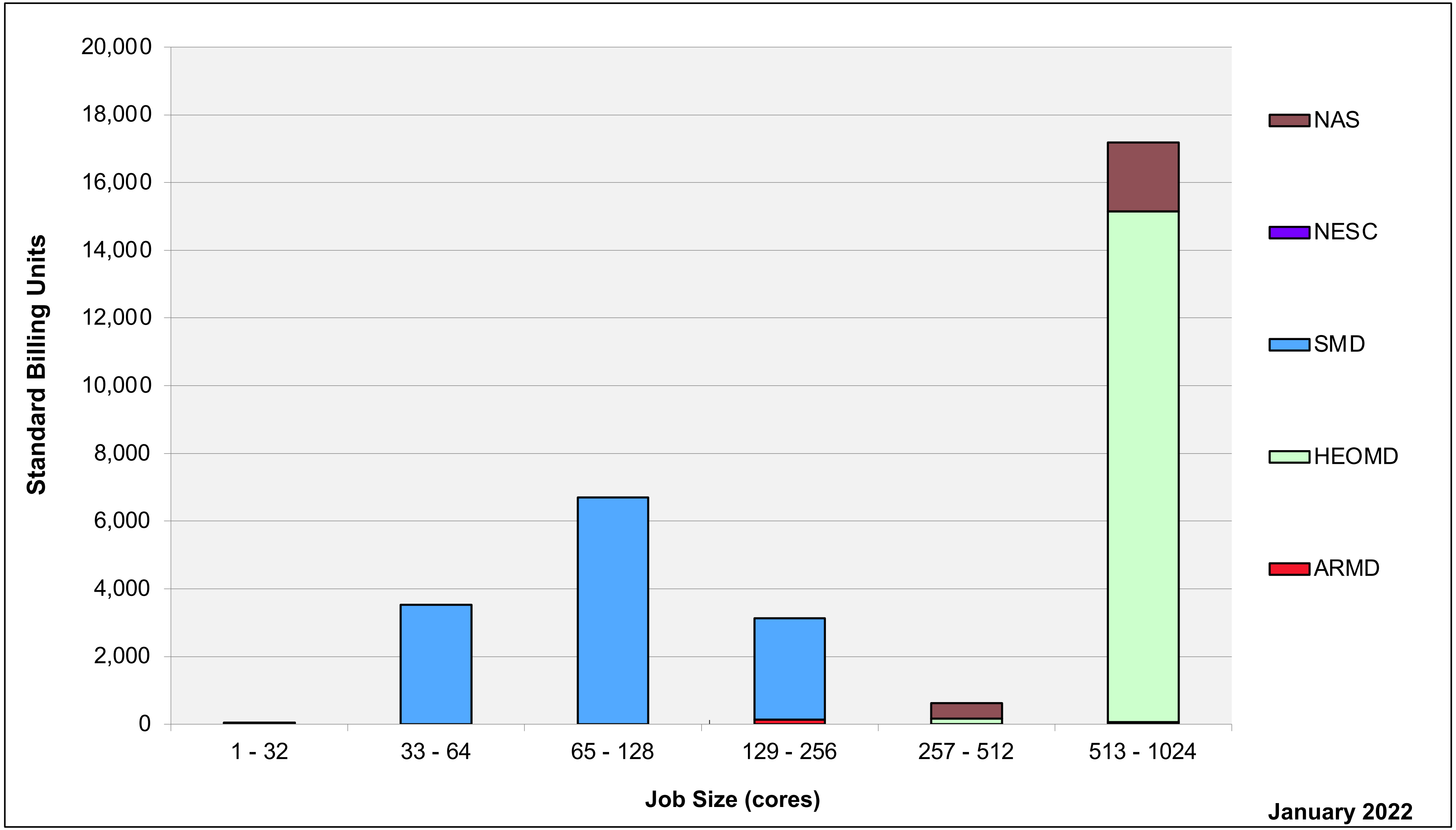
Endeavour: SBUs Reported, Normalized to 30-Day Month



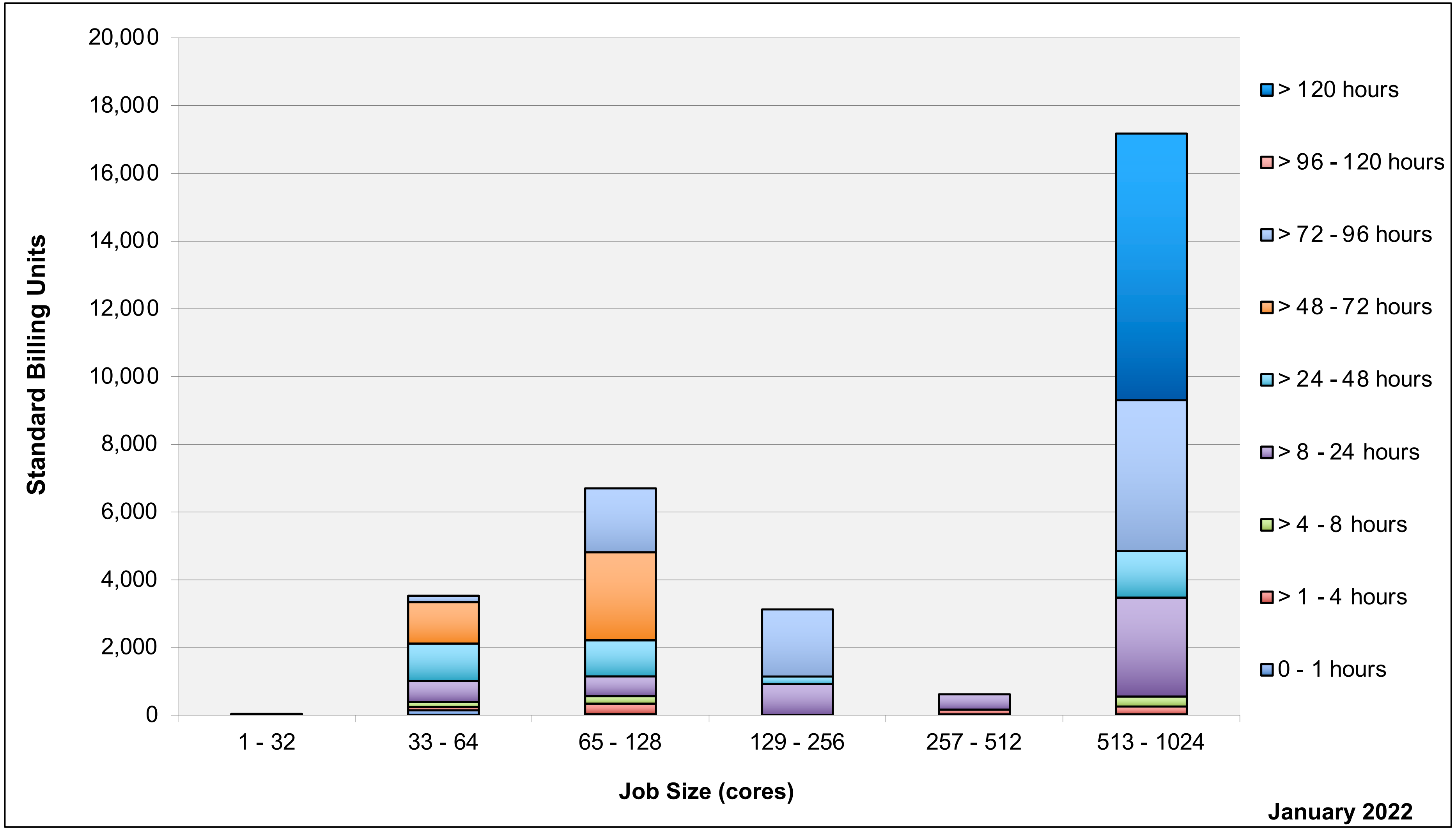
Endeavour: Monthly Utilization by Job Length



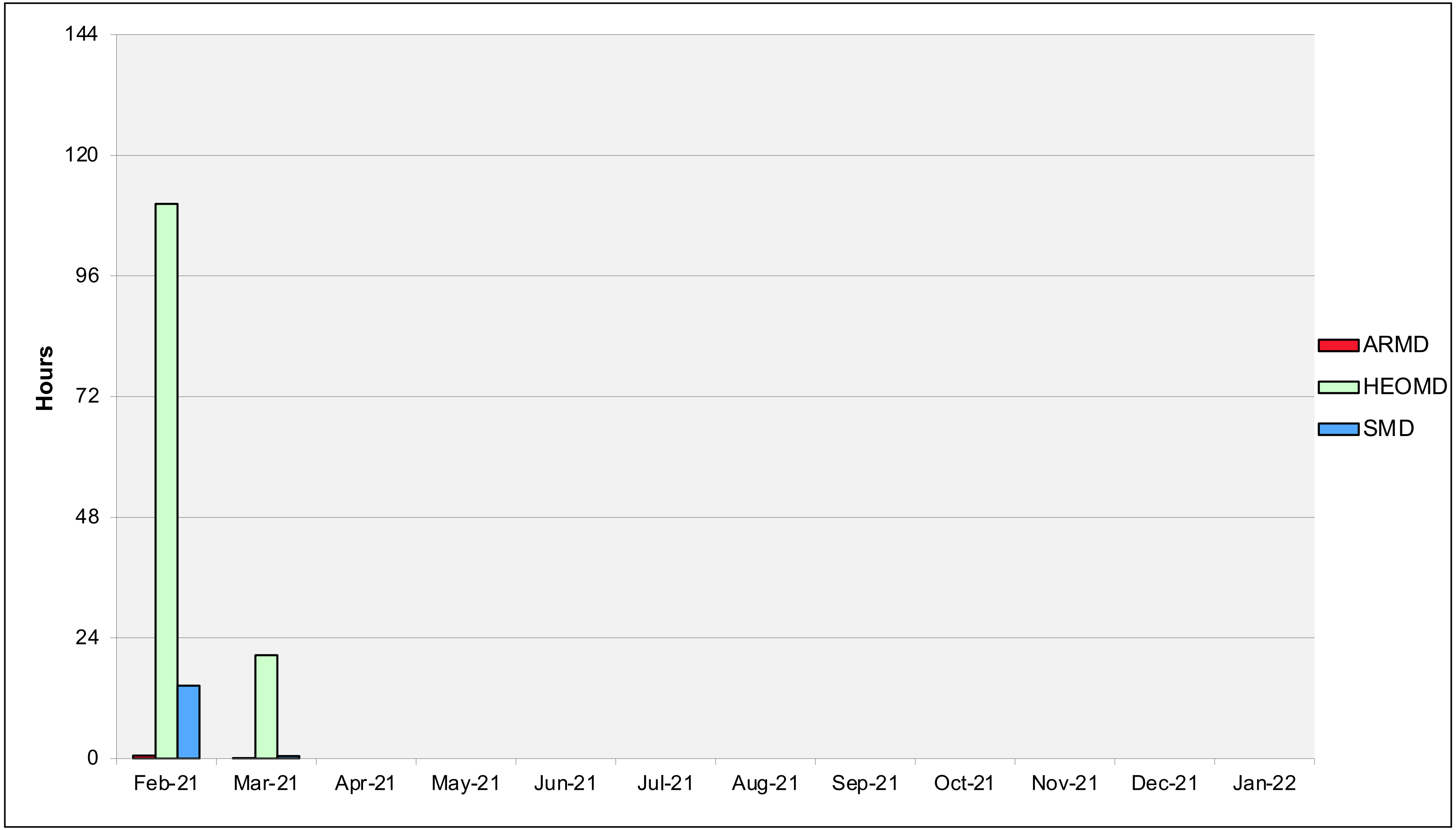
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor